UNIVERSITY OF SOUTHERN CALIFORNIA

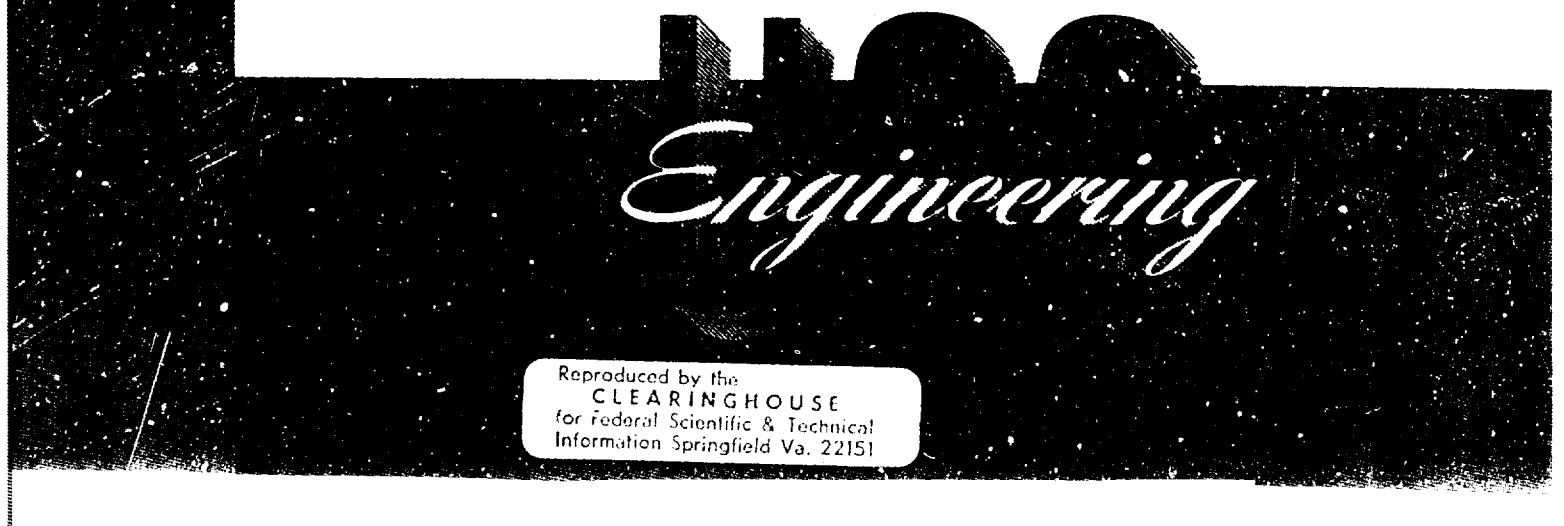
CONSOLIDATED SEMIANNUAL PROGRESS REPORT

NO. 10

Covering Research Activity During The Period

1 April 1969 through 30 September 1969

ELECTRONIC SCIENCES LABORATORY



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Prepared By
The
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APPENDIX

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1. SOLID STATE

1.1 SEMICONDUCTORS

1.1.1 Infrared Studies of Semiconductors

GK 10633, National Science Foundation
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W. G. Spitzer, L. Eggers, R. Eaglet, M. Levy, L. Skolnik, and W. Allred

Studies of several types of impurity--or defect--induced absorption, which have been discussed in earlier progress reports, are being continued. The specific projects are discussed in the sections which follow:

I. Vibrational Modes of Defects in GaP
W. G. Spitzer and W. Allred

Because of the technological importance of GaP as a luminescent material, considerable effort has been given to the study of the role of a variety of impurities in this material. We have studied the infrared absorption of doped material in the hope of identifying absorption bands introduced by the impurities. These bands arise from the modification of the phonon spectrum of the pure material by the presence of the impurity. In particular, under proper conditions of mass and force constants, modes can appear in which the vibrational energy is localized to the immediate vicinity of the defect.

A number of absorption bands have been observed and tentative assignments have been made on the basis of the known impurities present. In particular, a band at $\omega = 453\ cm^{-1}$ is attributed to Si_{Ga}

(silicon substitutional on a gallium site), one at 464 cm^{-1} to N_P or O_P, 443 cm^{-1} to Al_{Ga}, 569 cm^{-1} to $^{11}B_{Ga}$, and 592 cm^{-1} to $^{10}B_{Ga}$. Other defect bands are observed at 527 and 606 cm^{-1}. However, present experimental results are not sufficient to permit identification of the impurities responsible for these latter bands.

II. Band Edge Absorption in Lithium Diffused GaAs

R. Eaglet and W. Spitzer

Several investigations have been made of the infrared absorption of localized vibrational modes of defects in GaAs. Lithium compensation is used to inhibit the free carrier absorption which would otherwise mask the absorption. We have undertaken an experimental examination of the effects of Li compensation on the electronic density of states in impure GaAs.

Absorption and photoconductivity measurements have been made on two groups of samples: (1) Impure n-type GaAs samples taken from the same pulled ingot. These samples were given varying degrees of Li compensation (by varying the Li diffusion temperatures). (2) GaAs doped to various initial Si concentrations, which were exposed to identical Li treatment.

For these n-type samples, the effects on the absorption spectrum can be explained by Gaussian distributed donor and acceptor bands located just adjacent to the conduction and valence bands respectively. On these are superimposed exponential state density tails which extend from either band deep into the forbidden gap. The size of the Gaussian distributed impurity bands depends on the donor and acceptor concentrations, including the donor and acceptor configurations of the Li. The Gaussian bands can be accounted for by consideration of mutual coulombic effects between ionized donors as their concentration reaches a level where they are close enough to interact.

The exponential tails, which also exist without Li, have been

explained as due to disorder in the lattice, localized compressions and dilations due to incorporation of impurities, or an internal Franz-Keldysch effect due to charged impurities. The exponential tail states depend on the amount of Li incorporated in the following manner. The exponential slope, $d/d(h\nu)$ (ln α) decreases monotonically as the net impurity concentration of a given type increases. Therefore in identical n-type samples which were overcompensated to p-type by varying amounts of Li, those exposed to the highest Li diffusion temperatures have the lowest exponential slopes. In samples with identical Li treatment, but varying initial net donor concentrations, those with the highest initial donor concentrations have the highest exponential slopes.

Confirmation was accorded to interpretation of these measurements when the photoconductivity results were analyzed. Most photocurrent is due to transitions terminating in the unperturbed portion of the conduction band. Electrons in the merged Gaussian donor band played on a minor role. Hole current was not observed, even in samples which were over compensated to p-type in the dark. This is probably due to a large number of hole traps, and to a lesser extent, lower hole mobility relative to that for electrons.

III. Local Modes in Lithium Diffused, Manganese Doped GaAs

M. Levy, L. Eggers, and W. G. Spitzer

In some earlier work it was observed that lithium local modes were observed in p-type GaAs which was compensated by Li diffusion. The mode frequencies were dependent upon the specific acceptor impurity present and showed nearly the full isotope shift expected for a pure Li vibration. In both Mn and Cd doped material, three Li modes were observed and the simplest model which we could propose to account for the spectra was as follows: The Mn (or Cd) is substitutional on a Ga site i.e., Mn_{Ga} (or Cd_{Ga}). The compensating Li ion pairs with the acceptor in an interstitial site with four As nearest neighbors and the Mn_{Ga} + 5 Ga as second neighbors. The Mn_{Ga}-Li_i axis is in a < 100 > direction. This

model gave a reasonable semi-quantitative account of the observed spectra.

Dr. R. Title of IBM (Yorktown Heights, N. Y.) has recently made e.p.r. measurements of Li diffused GaP and GaAs. In both of these cases it was observed that the principal symmetry axis is in the <110> direction rather than a <100> direction. For GaP, Title proposed a defect consisting of Mn_{Ga}-Li_{Ga}-2 Li_i where the Mn_{Ga} and Li_{Ga} site are nearest neighbors on the gallium sublattice and the 2 Li_i are each in symmetrically arranged edge centered positions on the Ga sublattice. This defect is complicated in that it requires three Li's per center. The defect in GaAs is similar although it does show some differences.

There are at least two possible reasons for the differences in the two above interpretations. The first is that both methods are measuring the same defects and one of the interpretations is incorrect. There are some questions about both interpretations although the <110> symmetry axis of the e.p.r. work makes the infrared interpretation very suspect. A second possibility is that the two measurements are sensing different defects.

Measurements are now in progress which may help clarify the model. These measurements are infrared absorption of Mn doped samples some of which have been (1) compensated with Li at a variety of diffusion temperatures and (2) compensated with a variety Li isotopic abundances ranging from nearly pure ^7Li to ^6Li.

1.1.2 Materials Preparation

AF-AFOSR-69-1622A, Joint Services Electronics Program
PRF 4528-AC6, American Chemical Society
W. R. Wilcox, W. Allred, W. L. Paterson, V. Yip
and V. Kuo

The objectives of the materials preparation program are four-fold: (1) To do research on crystal growth phenomena and techniques; (2) To do research on purification of solids and materials used in preparation of solids; (3) To investigate the influence of preparative conditions on the properties of solids; and (4) To develop a crystal growth capability so that other researchers at USC needing materials will be able to prepare them, often with our assistance.

1.1.2.1 Crystal Growth

W. R. Wilcox, W. Allred, V. Yip

Further studies were carried out on the < 211 > twins formed during solution growth of KBr[1]. Twinning occurred when KBr reagent from Mallinckrodt Chemical Works was employed but not with reagent from the Baker Chemical Co. Addition of Na^{+} and Cl^{-} in substantial amounts induced twinning, but Fe^{+++}, Pb^{++}, BrO_3^{-}, $SO_4^{=}$ ions did not. A model explained many features of the twinning by showing that (1) the composition plane would be stabilized by slightly smaller cations and anions; (2) twinning produces an angular step analogous to a screw dislocation; and (3) if the composion plane is (211), then the sum of the thickness of the wings on one side must equal that on the other (which it does not experimentally). Further investigation is underway, including an analysis to determine the impurity content of reagents from the two suppliers.

Equipment has been assembled for a (hopefully) quick experiment to see if adsorption of radiotracer Te can be detected on the surface

of GaAs following growth and dissolution in Ga. If results are positive, then we should be able to see if the adsorption is preferential, as hypothesized in most of the proposed mechanisms for the well-known facet effect.

Apparatus is being assembled for an investigation of the travelling heater method of growing mixed III-V crystals.

Assistance was provided for the study on the effect of dopant interactions on their distribution coefficients during horizontal boat growth.[2] The following crystals have been grown in our laboratories for research at USC since March 1969: GaAs, InSb, $NaNO_3$, $NaClO_3$, Si.

Several papers were published and presented during this report period[3-8].

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1.1.2.2 Movement of Inclusions in the Centrifuge

W. R. Wilcox

The theory of movement of solvent inclusions in a centrifugal field was developed[1]. Experimentally, it was found that aqueous inclusions in KI moved inward at about 0.05 mm/hr. in a field of 210,000 G at room temperature. Higher rates were observed at 5°C, while the inclusions moved outward at 40°C. Agreement between experiment and theory was within experimental error and uncertainty in parameters required in the theory. A paper describing the results is in preparation. No further work is planned.

Reference

1. W. R. Wilcox and P. Shlichta, "Movement of Inclusions in Crystals by Centrifugation", International Union of Crystallography, Stony Brook Meeting, Aug. 1969.

1.1.2.3 Pushing of Foreign Particles by a Freezing Interface

V. Kuo

Foreign particles are pushed by a freezing interface up to a critical freezing rate V_c, above which the particles are trapped. Trapped particles are not only sources of impurities but can induce defects such as dislocations and twinning. V_c has been found to be a function of the type of particle and the material freezing, although no way is known for predicting it[1]. A program has been intiated to investigate the effect of temperature gradient, purity, and external force on V_c. Experimental apparatus has been constructed and some experimental results are expected within the next six months. Eventually, we also plan to investigate the relation between V_c and the effectiveness of the particles as heterogeneous nucleation catalysts for the melt.

Reference

1. D. R. Uhlmann, B. Chalmers, and K. A. Jackson, J. Appl. Phys. 35, 2986 (1964).

1.1.2.4 Silicon Nitride

W. Paterson

Charge storage in vapor-deposited silicon nitride films can be used in memory and logic devices.

Exploitation of this phenomenon is hampered by lack of understanding of the mechanisms involved. We plan to elucidate certain features by studying the effect of certain impurities on the properties of these films. Design of the deposition system and measuring instruments is in process.

1.1.3 Investigation of Semiconductor Phenomena Using Metal-Semiconductor (Schottky Barrier) Contacts

AF-AFOSR 69-1622A, Joint Services Electronics Program

C. R. Crowell V. L. Rideout G. I. Roberts,
C. L. Anderson and M.M.E. Beguwala

A. Background

This research consists of a continuing theoretical and experimental study of physical phenomena associated with current transport, charge trapping, interface effects and avalanche multiplication using metal-semiconductor (Schottky barrier) contacts. The following summary of the work in this area provides a perspective on the projects completed during the past six months and those in progress.

B. Current Transport

1. Theory

The normalized theory for current transport in metal-semiconductor (Schottky barrier) contacts of Crowell and Rideout[1] has been extended to include the effects of image force rounding of the otherwise parabolic potential energy barrier.[2] Quantum-mechanical reflection of carriers near the top of the barrier is included in the theory through the use of Kemble's formulation which incorporates the WKB tunneling into a transmission probability applicable to energies both greater than and less than the barrier energy. Thermionic and thermionic-field (tunnel) emission are analyzed in a normalized formulation to yield the current (I) versus voltage (V) relationship. The technique of normalization leads to a description of current transport in terms of significant parameters that are functions

of bias, temperature and donor concentration. This simplifies the application of the theory to practical situations.

In comparison with current transport models that neglect image force lowering[1,3], the present theory[2] shows that inclusion of image force leads to a significant increase in the predicted magnitude of the current density. When thermionic emission dominates the conduction process, a modest increase in the diode n value also results (note: the n value is the inverse slope of the semilog I versus V characteristic). The present theory with image force is also of value in explaining reported discrepancies between barrier heights deduced from I-V, C-V and photo-threshold analyses.

Application of the present thermionic-field theory to cases of thermionic dominated conduction (i.e., to situations where quantum-mechanical tunneling and reflection may be considered as a perturbation on thermionic emission) is facilitated by defining the Kemble transmission probability in terms of a characteristic transmission energy. Because of the similarities between thermionic emission at higher temperatures and the photoemission process, the characteristic transmission energy can also be used to estimate the magnitude of the perturbation due to tunneling and reflection on the photoresponse characteristic. Theoretical analysis of the photoresponse characteristic is now in progress.

2. Experiment

The high vacuum electron beam evaporation system is operational and is being used routinely to provide gold and platinum Schottky barrier contacts on silicon and gallium-arsenide substrates. A mechanical-chemical polishing technique using the Syton colloidal silica polishing solution has been developed to provide high quality polished surfaces for silicon. A chemical surface cleaning process and a chemical spin-etching technique have also been developed for silicon. Platinum-silicon contacts have been alloyed to produce platinum silicide-silicon contacts. Platinum silicide is an intermetallic alloy whose barrier height on n-type silicon is approximately 0.85 eV[4]. The silicide contacts yielded diodes with lower edge leakage currents and more nearly ideal current-voltage characteristics (i.e., lower n values) than either platinum or gold contacts on the same silicon substrates.

I-V C-V and photothreshold measurements will be performed on the silicide diodes in an effort to confirm various aspects[5] of the normalized current transport theory[2].

C. C-V Relationship in Metal-Semiconductor Contacts

This study is intended to determine the effect of deep lying impurities in semiconductors on the capacitance versus voltage (C-V) relationship of metal-semiconductor diodes. A theoretical analysis of the effects of deep impurities on the C-V relationship at both low and high frequencies of bias modulation has been completed[6]. Low frequencies are those at which all deep lying impurities respond to the applied AC bias modulation and high frequencies are those at which one or more of the impurities may not respond. This analysis predicts that an energy level spectroscopy of deep impurity levels in the semiconductor may be obtained from the low frequency C-V relationship. Additional information about the charging times of ionized deep impurity levels may be obtained from the C-V relationship as a function of frequency.

Schottky barrier diodes are being fabricated on silicon substrates intentionally doped with selected deep lying impurities. The C-V relationship of the diodes will be measured as a function of frequency. The energy levels of the deep impurities obtained from the C-V data will be compared with the published values of energy levels measured by other means (i.e., by optical and thermal techniques). In addition, the charging times of the ionized deep levels, which are presently unknown, will be determined.

Further refinement of the C-V theory will also be undertaken. In particular, the effect of a nonspatially constant imref on the energy level spectroscopy will be considered.

D. High-Field Current Transport and Avalanche Multiplication

Previous work by Crowell and Sze[1] predicting the temperature dependence of the avalanche coefficients of charge carriers in semiconductors

has not received a detailed experimental investigation. We plan to investigate this phenomenon by photoexcitation of the avalanche inducing carriers over the potential energy barrier of a metal-semiconductor contact. This technique allows the injection of a selected carrier type (i.e., majority carriers) into a predetermined electric field distribution at a particular physical location in the semiconductor. This technique, if employed in the pre-avalanch region, also allows a measurement of the high-field drift velocity of the carriers. A near-infrared spectrometer system has been prepared for these measurements. Theoretical work in progress has yielded a criterion for the relationship between the velocities of the carriers resulting from a pair production process at threshold. The relationship allows a systematic determination of the threshold energy for pair production for any semiconducting material whose band structure is known.

E. Majority Carrier Diffusion Study

A theoretical study of the contribution of majority carrier diffusion to the magnitude of the diode n value (i.e., the slope of the semi-log current versus voltage relationship) is presently underway. We have solved Schottky's diffusion equation[8] without the usual approximations to obtain the current-voltage relationship and a normalized universal computer plot of n value versus band bending. A special case of diffusion equation derived by Crowell and Sze[9] was also analyzed in a normalized fashion, and the diode n value obtained as a function of dimensionless parameters. These include the band bending in units of kT and the ratio of recombination velocity to what may be defined as a Debye diffusion velocity V_D ($V_D = kT/2q\,L_D$, where L_D is the Debye screening length). The n values obtained from the two theories were compared for various values of band bending. The ratio of the saturation current to the thermionic current was also computed for both models. In addition, the effect of Crowell and Sze's diffusion equation for the imref was analyzed. This resulted in a general normalized equation for imref and an estimate

of the forward and reverse bias limits for application of the assumption of a constant imref.

From the above analysis it was determined that the contribution of diffusion to the n value of a metal-semiconductor diode is much less than previously thought. The maximum predicted n values range from 1.005 to 1.040 for values of band bending ranging from 50 to 10 kT. The imref in the semiconductor was found to be relatively constant over a large portion of the depletion layer even for moderate values of forward bias. The variation in imref was found to occur primarily over the 10% of the depletion layer width nearest to the metal-semiconductor interface.

F. Impurity Profile Determination

A number of schemes have been reported for using $d(1/c^2)/dV$ versus 1/C to determine semiconductor doping profiles, among them being one by Copeland.[10] Copeland's scheme uses a measurement of the fundamental and second harmonic voltages generated within a Schottky diode by a constant current rf signal superimposed on a dc bias. The system is simple to operate but requires a relatively complex filter to assure isolation of the diode from the second harmonic generated in the r-f source and isolation of the voltmeter used to read the second harmonic voltage from the rf signal at the fundamental frequency. We propose that an r-f constant current source also be used but that this source be gated at a low audio frequency. This will generate an audio frequency voltage similar in magnitude to the rf second harmonic voltage measured by Copeland. The leakage impedance requirements of this alternative scheme are more stringent than Copeland's but the system will be broad-band in the rf spectrum and thus will not require critcal tuning. A preliminary circuit design has been completed for this task.

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1.1.4 Radiative Recombination in Semiconductors

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Background

The long-range aim of this proposal is the development of efficient solid-state visible light emitters, as individual lamps or display panels, to be the interface coupling between modern solid-state circuitry and the human eye. Such devices should emit efficiently in the visible spectrum when driven by low DC voltages and their technology should be compatible with present state-of-the-art integrated circuit technology. These requirements can be met by wide-bandgap semiconductors, some of which are already being used for this purpose.

Our concern is with the preparation and basic properties of such materials (crystal growth, defects, band structure, transport, and optical characteristics), with their luminescent properties (recombination of minority carriers at various defects), and with electrical injection of minority carriers (p-n junctions, tunneling structures,...).

We are currently working with GaN, ZnS, AlP and Si (the latter, while not a wide-gap material is a good material in which to study radiative recombination processes because its properties are so well understood) and hope to expand to some wide direct bandgap alloys (e.g., Ga-InP) as well as a near infrared emitter (InAs, InAs-Sb) in the near future.

GaN

We have shown that the solubility of nitrogen in gallium is extremely small even at 1200°C and up to 5 atmospheres. Hence growth of GaN from the melt or from Ga solutions would require a high temperature,

high pressure growth apparatus. We do not feel such an investment in time, effort and money is appropriate at this time. Instead, we have been investigating several vapor growth techniques for several reasons: (1) The containment and contamination difficulties associated with melt or solution growth are avoided. (2) Both Ga and N are easily obtained as vapor species. (3) Vapor growth may be either self-nucleating or the material may be grown epitaxially on an inert substrate. Although self-nucleation usually results in small crystals, the crystals tend to be strain-free, an important desideratum for observing sharp lines in emission or absorption spectra. The sample size needed to fill the aperature and slit of our high resolution spectrometer (with 5:1 image magnification) is only $\sim 0.5 \times 0.01$ mm. Hence, we can accept small crystallites for this phase of our work. Large-scale epitaxial growth which now appears feasible (see below) will supply crystals for some of our other interest including transport measurements, and device fabrication.

In the past few months we have (first) investigated the vapor phase reactions between either pure Ga or Ga_2O with N_2 or NH_3 and (second) found a more useful approach by using a halide vapor carrier for the Ga.

In the first approach, our best results have been obtained by volatalizing pure Ga from a quartz boat in a H_2 stream at $\sim 1100^{\circ}C$. Here Ga has a vapor pressure of ~ 0.04 torr. We believe that the Ga is transported as a pure Ga species for the following reasons. First, the weight loss per unit time is less than the maximum weight loss rate calculated from the known vapor pressure of Ga even assuming an accommodation coefficient of unity. Second, transport as the vapor species Ga_2O has been ruled out by noting that the transport rate is not effected by increasing or decreasing the H_2O contamination in the carrier gas.

The Ga/H_2 stream is injected through a capillary tube (to prevent back-diffusion) into a reaction chamber through which NH_3 flows. The Ga stream is mixed with the NH_3 at the high-temperature end of a

thermal gradient. Crystallization occurs at temperatures $\sim \bar{<} 800^{\circ}C$. To date we have obtained platelets and ribbons up to about 1/2 x 1/2 mm. This size is just barely suitable for our optical work. X-ray powder patterns of the crystals indicate that they correspond to the Wurzite structure, with the lattice parameters of GaN. Although grown in an all quartz apparatus no x-ray lines attributable to the various forms of Ga_2O_3 and SiO_2 could be detected. In fact, all the observed diffraction lines could be assigned to GaN. The crystals are also optically transparent in the visible.

Preliminary results indicate that GaN can be grown epitaxially by this method on (111) Si wafers placed at the upstream edge of the nucleation region.

Although growth by this method is slow because of the low vapor pressure of Ga at these temperatures we have demonstrated that crystal growth does occur and leads to crystals (barely) large enough for optical examination at present.

Previously, we reported on a brief investigation of the closed-tube transport of microcrystalline GaN by a halide carrier (I_2 and Cl_2) in a thermal gradient. Although a volatile Ga halide was formed and transported to the cold end of the tube, the other vapor species produced was molecular N_2 which did not react with the halide in the cold zone. Hence the net result was the deposition of metallic Ga in the cold zone and the formation of gaseous N_2.

Hence, we converted to an open tube system (for convenience) transporting Ga as a halide (by reacting pure Ga with HCl in a H_2 stream), but reacting the halide species with NH_3 downstream. Care had to be used to avoid any direct contact between the NH_3 and the hot Ga metal or else the Ga would rapidly be converted to microcrystalline GaN by the direct liquid-vapor-quartz catalyst mechanism described previously. The overall method works, but not as originally envisioned. There are several stable vapor chlorides of Ga, depending on temperature and pressures:

$GaCl_3$, $GaCl_2$ and GaCl. One of them is formed predominently in the hot zone where the Ga boat is kept. At a given NH_3 pressure downstream, GaN is produced only when the temperature is considerably below the generation temperature (800^o vs. 1100^o) so that the generated halide species must disproportionate before its reaction with NH_3.

Self-nucleated GaN crystals grown by this method (on quartz) are small (~ 0.1 mm) but are otherwise almost perfect-transparent, good crystal habit and strain-free. Attempts at epitaxial growth (on quartz, Si, GaAs and sapphire) have been partially successful. Only polycrystalline layers have been grown. Our previous growth attempts using Ga_2O had shown that the present growth conditions are ideal for forming β-Ga_2O_3. From this information and from careful examination of the GaN films we believe that a small oxygen contaminant (as O_2 or H_2O) is causing local nucleation of Ga_2O_3 and thus preventing the GaN layers from growing coherently. We are therefore presently engaged in improving our gas purification system to reduce the O_2 and H_2O content.

Other Projects

No progress has been made on the optical and luminescent investigation of the AlP crystals grown earlier because of the lack of manpower.

The investigation of the possibility of moving the Fermi level in ZnS over a wide range at high temperatures (thus producing p-type ZnS) by annealing at high pressures of Zn or S vapor has been successful except for a lack of quantitative reproducibility, which we suspect is due to the fact that we lack control over the starting material. (We do not grow the ZnS). We are currently ascertaining whether surface effects are causing some of the lack of reproducibility. If these effects can be controlled, we will try using doped crystals in these anneal cycles in the hope of obtaining crystals that are p-type even at room temperature.

The search for isolated pair lines in Si and the investigation of the mechanism of the efficient Cu green luminescence in ZnS has been delayed due to instrumental difficulties. In addition, the latter project

would be greatly expedited if a CW UV laser (in the 2500-3300 Å) region were available. We are therefore currently proposing to buy or build a frequency doubled cw argon laser for this purpose.

Two other projects are now being started: (1) a cooperative venture with Dr. J.M. Whelan in which we would investigate the fluorescent, electroluminescent and laser properties of InAs and InAs-Sb alloys he would prepare in the hope of preparing efficient light emitting diodes in the 3-6 micron region in the infrared. (2) Evaporation of CdS together with possible shallow acceptor impurities onto CdS substrates held at low temperatures to form doped amorphous CdS layers, which upon subsequent (or simultaneous) annealing might yield p-type CdS.

1.1.5 Electron Probe Analysis of Semiconductors

AF-AFOSR-68-1414, Air Force Office of Scientific Research

D. B. Wittry, N. Gardner, J. H. McCoy, H. C. Marciniak, J. Potosky, T.S. Rao Sahib, P.A. Sullivan, and R. Tamura

1.1.5.1 Cathodoluminescence of Semiconductors

H. Marciniak and D. B. Wittry

Tests of the ultrahigh vacuum electron probe instrument have been continued. Using a single electron lens, sample currents of about 0.2 μA at 20 kV were achieved in a focal spot approximately 10 microns in diameter. In these initial tests, pumping periods have been relatively short (about 2 hours maximum) and the lowest pressure achieved has been about 7×10^{-7} Torr. After prolonged pumping and low temperature bakeout much lower pressures should be attainable. The Spex monochromator and Brower optical detection system have been checked with the new probe column using the cathodoluminescence of Benitoite.

Measurement of the cathodoluminescence of p type GaAs at various temperatures is now being investigated. It is also planned to study cathodoluminescence of GaP and of mixed crystals in the GaAs-GaP system. Initial investigations of $GaAs_{1-x}P_x$ were done in this laboratory several years ago[1] but were not completed because the standards used for determining the composition with the electron probe microanalyzer were subsequently found to be inhomogeneous. In the previous work only spectra at room temperature could be recorded because of contamination of the

specimen. With the new probe column, it will be possible to obtain spectra at temperatures down to 20°K and this should contribute much to understanding the optical transitions in specimens of different phosphorus concentration.

The original electron probe microanalyzer has been modified for secondary electron detection and higher resolution in the SEM mode. This instrument will be used for room temperature cathodoluminescence measurements and correlation with the composition determined from electron probe microanalysis.

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1.1.5.2 Electron Beam Modulated Optical Properties of Semiconductors

J. H. McCoy and D. B. Wittry

In the previous semiannual report, investigations to determine the mechanism for electron beam modulated reflectance of semiconductors were described, and an electron beam modulated reflectance (EBMR) spectrum of GaAs was shown. Further experiments have now been conducted including electron beam modulated absorption and reflection at energies less than the band gap energy, and measurements of EBMR spectra from other semiconductor materials. The semiconductor materials investigated to date include Si, Ge, GaAs and GaP. It seems clear from the investigations conducted up to now that the EBMR effect is due to temperature modulation. While it might seem that EBMR is a very elaborate way to do thermoreflectance there are important advantages in the EBMR technique over other modulated-reflectance techniques. These are the following: (1) no special sample preparation is necessary, (2) modulation at higher frequencies is possible than can be obtained with usual methods of thermal modulation, and (3) the amplitude of the modulation can be much larger than with usual methods of thermal modulation. Because of the large modulation amplitudes, the EBMR technique has shown some details not previously seen in the modulated reflectance spectra of semiconductors. Also because of the large modulation possible, the EBMR technique should also be applicable to metals.

The results of this work are described in detail in the Ph. D.

thesis of J. H. McCoy and a paper summarizing the results is in preparation.

1.1.5.3 The X-Ray Continuum from Thick Targets

T. S. Rao Sahib and D. B. Wittry

According to the theoretical treatment of Kramers[1,2], for a fixed wavelength and beam voltage the intensity of the X-ray continuum should be directly proportional to the atomic number of the target.

If the intensity of the X-ray continuum as produced and measured in an electron probe microanalyzer is found to verify the above prediction after correction for absorption and atomic number effects, then this would provide additional confidence in the commonly accepted values of mass absorption coefficients and the general procedures for applying corrections to experimentally observed intensities. Such a verification would also provide a means of adjusting the mass absorption coefficient for any element whose corrected continuum intensity deviates from the predicted proportionality with atomic number.

In the present study an EMX modified to EMX-SM microanalyzer was used. The beam voltage was kept constant at 30 kV. X-ray continuum intensity as a function of atomic number was measured using pulse height discrimination at wavelengths of 1.998 Å, 3.956 Å and 7.981 Å corresponding to the Sm L β_1, Cd L α_1, and Al Kβ_1 lines respectively. Beam current was measured with a Faraday cage. Nineteen elements ranging in atomic number from 12 to 92 were examined.

Absorption and atomic number effect corrections were made under the following assumptions:

1) The cross-section for production of the continuum is independent of the energy of the electrons.

2) The spatial distribution of excitation for the X-ray continuum is the same as for characteristic X-rays.

3) The mass absorption coefficient is known. Heinrich's values of μ/ρ for the Sm $L\beta_1$, Cd $L\alpha_1$ and Al $K\beta_1$ lines were used.[3]

4) Measurements at 1.998 Å and 3.956 Å were corrected for absorption using Philibert's formula for $f(\chi)$ with Duncumb and Shields' voltage dependence of $f(\chi)$[4] and Heinrich's coefficient for voltage.[5] At 7.931 Å, absorption corrections were made following the procedure of Andersen and Wittry.[6]

5) The atomic number correction is calculated from eqn. (10) of Duncumb and Reed[7] using $E_k = 12.393/\lambda$, $\lambda = 1.998$ Å, 3.956 Å, 7.981 Å, together with assumption (1) above and Bishop's data[8] for backscatter coefficient η.

At 1.998 Å, the results obtained are in general very similar to those obtained earlier[9] using the EMX microanalyzer before the SM modification. With the exception of Fe and U, the linear dependence of continuum intensity on atomic number is obeyed by the remaining elements. The intensity from Fe is about 35% too high and is due to the proximity of the Fe $K\alpha_1\alpha_2$ line which has its peak at 1.9373 Å. This was verified by repeating the experiment at 2.103 Å (Mn $K\alpha_1\alpha_2$). In this case the continuum intensity from Fe follows the linear variation. The intensity from U is about 15% too low at 1.998 Å, but is very close to its expected value at 2.103 Å. No ready explanation can be given for this fluctuation in the intensity. The anomalous low value of intensity from Mn reported elsewhere[9] is very probably due to that measurement having been made on a region of the Mn standard which was not perfectly flat. With the improved optical resolution now available, the possibility of such errors has been greatly reduced in the present series of measurements.

At 3.956 Å, the continuum intensity is again found to vary in a linear manner with atomic number. However, the corrected intensities from Au and Bi are about 17% too high, and from Pb about 45%. Since these elements lie in the region of the M absorption edge, it is possible that the discrepancy is due to uncertainty in the value of the absorption coefficient.

In order to preserve the intensity/atomic number linear dependence, the following values of absorption coefficient are required: Au, 1350.4; Pb, 996.0; Bi, 1276.9. The values of the absorption coefficients according to Heinrich's tables are: Au, 1725.1; Pb, 1952.7; Bi, 1760.8. Thus, the technique suggested by this study might be used to estimate μ/ρ for an element at any particular wavelength. If the X-ray continuum excitation is distributed in the same manner as the characteristic X-ray excitation, as seems to be the case, then the accuracy of the estimates of μ/ρ made above is limited by the accuracy of the Philibert $f(\chi)$ formula for $f(\chi) \approx 0.4$, this being approximately the magnitude of the absorption correction required for the above three elements.

At 7.981 Å, the $f(\chi)$ values range from 0.1 - 0.3, and hence the Andersen and Wittry[6] absorption correction function was used. If the lower $f(\chi)$ curve is used (Fig. 5 of Ref. [6]), then the intensities for atomic number $Z \geq 26$ appear to be overcorrected. A considerable improvement in linearity up to $Z = 51$ can be effected if the upper $f(\chi)$ is used for atomic numbers $Z \geq 26$. This would appear to be additional evidence for a spread in the $f(\chi)$ curve for $f(\chi) < 0.5$. In order to reduce the possibility that radiation from the instrument due to backscattered electrons could be contributing to the measured X-ray intensity, the experiment was repeated with a Mylar shield placed in the bore of the objective lens just above the specimen. The presence of the shield did not result in any significant improvement in linearity of the corrected intensities. Also of interest are the consistently high intensities obtained from Mn and Zn. These elements have a corrected continuum intensity about 2.5 times greater than expected. Further investigations on these two elements need to be made.

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1.1.5.4 Compound Semiconductor Surface Studies

P. A. Sullivan and D. B. Wittry

The studies of slow transient cathodoluminescence described in the last report are continuing toward two goals: preparation of clear reproducible surfaces and measurement of surface potential variations associated with electron beam induced adsorption and desorption.

Preparation of smooth surfaces on compound semiconductors (especially the more ionic compounds) has received little attention in the literature. Previously used[1,2] and new chemical polishing techniques are being studied.

The electron optics of an EMX microanalyzer is being modified to function as a scanning mirror microscope[3,4,5] which will make it possible to study contact potentials, conductivities, surface charges, and topography of compound semiconductor surfaces. The slow transients in certain properties of several compound semiconductors[6-10] has been

attributed to desorption of oxygen. With the mirror electron microscope it is hoped that measurements can be made of surface potential variations associated with electron-beam-induced sorption effects and that these effects can be correlated with changes in the surface recombination velocity for minority carriers. In these measurements the intensity of cathodoluminescence will be used as an indication of changes in surface recombination velocity.

In the initial experiment the vacuum conditions will be the same as normally used in electron probe microanalyzers or scanning electron microscopes. However, it is apparent that subsequent experiments will require better vacuum than presently available, better control of initial surface condition, and methods for studying the nature of atoms or ions.

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1.1.5 Quantitative Electron Microscopy

GK 3904, National Science Foundation

R. Gauldin and D. B. Wittry

This project involves investigation of several possible methods of obtaining quantitative information from transmission or scanning electron microscopes. Among the possible sources of quantitative information from electron beam interactions with solids, the ones that have received little attention until recently are Auger electron emission and characteristic energy losses of transmitted electrons. The importance of Auger electron energy analysis in scanning electron beam instruments was pointed out in a recent review paper[1] and the use of electron spectrometers with such instruments has already been reported[2,3]. While one of the original goals of this project was to explore the possibilities of obtaining quantitative information in scanning electron microscopy using energy analysis of Auger electrons, it appears that this approach is being investigated in many other laboratories. Because of the great interest in Auger electron spectroscopy, it appears that the efforts in our laboratory could be more profitably spent emphasizing the second aspect of the proposed research, namely the study of energy losses incurred by electrons transmitted through thin films.

In a paper now in press, various approaches to instrumentation combining electron spectrometry with transmission electron microscopy were discussed and a simple electron spectrometer for use below the camera chamber of a transmission electron microscope was described[4]. Preliminary results obtained with this spectrometer system are described in another paper in press and indicate some of the possibilities of the "selected area electron spectrometry" technique[5].

During the past 6 months the design of a similar spectrometer for use with the Hitachi HU 125 instrument was completed and the construction of the spectrometer was initiated. Electronic circuitry for using the signal averaging device (CAT) as a multichannel scaler for recording the

electron signals on paper tape was also developed. With this approach, it will be possible to record the transmitted electron signal digitally for subsequent computer processing.

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1.1.7 Epitaxial GaAs Films and Ohmic Contacts

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GK 2908, National Science Foundation

J. M. Whelan

Development of a technique for growing GaAs epitaxial films from Ga solution has now progressed to the point where the films are competitive with vapor grown films with respect to planarity and smoothness. Substrate orientation and the temperature gradients during growth are the critical factors responsible for the improvements. This epitaxial technique has been extended to the growth of $Ga_xIn_{1-x}Ps$ and $GaAs\ Sb_{1-x}$ films on GaAs substrates. Substantial shifts of the energy gaps of these films, relative to that of GaAs, have been achieved. Choice of substrate orientation is limited to either $(\bar{1}\,\bar{1}\,\bar{1})$ or $(1\,1\,1)$ for the alloys.

Liquid solution growth of GaAs and its alloys is most commonly done under a H_2 atmosphere to reduce the solubility of oxygen in solutions. The utility of calcium oxide doped zirconia cells to monitor H_2O concentrations down to 2 ppm in the H_2 has been demonstrated.

A sputtered-alloyed Au-Sn contact to n-type GaAs has been developed. It is characterized by having a contact resistance less than 10^{-5} ohm cm^2 to N^+ GaAs, a penetration depth $\lesssim$ 1000 A and suitable for ultrasonic or thermal compression bonding. Suitable alloy temperatures are from 350° to 375°. This contact is one feature of a GaAs field effect transistor being developed using solution grown films.

1.2 QUANTUM ELECTRONICS AND LASERS

1.2.1 Computer Studies of High Intensity Beam Propagation

N00014-67-A-0269-006, Office of Naval Research
AF-AFOSR-69-1622, Joint Services Electronics Program
W. G. Wagner

The availability of lasers has stimulated great interest in the nonlinear interactions of optical electromagnetic waves with matter. Early attempts to understand some of these interactions on a quantitative basis led to the conclusion that extensive work on the distortions of the beam resulting from nonlinear terms in the wave equations are of major importance. As in all systems governed by nonlinear equations, the variety of phenomena is extraordinarily full, and we have chosen to concetrate our attention on questions relating to the stability of the propagation of high intensity beams.

Propagation characteristics related to density and thermal variations in the medium have been discussed by Brueckner and Jorna[1], Kroll[2], Wagner[3], Herman and Gray[4], Raizner[5], Akhmanov et al.[6], Whinnery et al.[7], Inaba and Ito[8], and Carmen and Kelley[9]. For laser pulses of long duration, thermal effects dominate the effects of electrostriction and of molecular reorientation, and the studies of the influence of heat deposition upon the propagation of a high intensity electromagnetic beam can be classified into two groups. The first four of the referenced investigations often are described as studies of stimulated Rayleigh scattering, and the remaining studies usually are referred to under the topic of thermal blooming. The stimulated Rayleigh scattering papers are concerned with the growth of instabilities as a uniform electromagnetic wave propagates through a fluid, and their scope is limited to an examination of linearized equations describing laser propagation and the density and thermal fluctuations in the fluid. The remaining set of referenced papers concentrate on gross effects of thermal deposition, and the

principal features of beam propagation at intermediate intensities are rather well understood through such work. Experiments have not demonstrated yet the importance of stimulated Rayleigh scattering, but existing experiments should not have detected the instabilities because of the long path lengths required for their amplification.

There have been some suggestions that the instability calculations and the thermal blooming calculations are merely two different theoretical approaches to describing the same phenomenon. This does not appear to be the case because the scale length for instability development does not depend critically upon the width of the beam, whereas the scale length for gross thermal distortions of the beam is severely dependent upon the beam radius. More importantly, the instability analyses lead to the suspicion that the propagation state may never reach a temporal steady state, whereas almost all work on thermal blooming suggests that the final state is time independent. To understand better the possible importance of the distinction, an analogy with hydrodynamic terminology may be helpful. In that analogy, the thermal blooming studies presume that the flow will be laminar, whereas the instability analyses suggest the flow might be turbulent.

Many experimental and theoretical investigations indicate that fluid motion, convective in nature, exerts a pronounced influence on the propagation of laser beams. It seems reasonable that turbulent fluid motion would also have an important influence if it existed. The possibility exists that the instabilities associated with stimulated Rayleigh scattering could lead to driven turbulence in the fluid. Such turbulent fluid motion may be amplified rapidly from velocity fluctuations always presented in the fluid.

Our efforts to understand the coupling of the instabilities to fluid motions has been entirely theoretical in nature during the past period, and are only the beginning of both a theoretical and experimental program to understand the nature of the state of propagation implied by the instabilities.

We have been impressed by the importance of obtaining more information on stimulated Rayleigh scattering than can be derived from linearized analyses, which yield very little qualitative insight. The gross calculations of thermal blooming, and of beam bending and distortion associated with fluid flow, produce much qualitative insight, but they cannot account for the effects indicated by the instability analyses. Therefore, another approach to the propagation problem is required, which can incorporate the feedback effects of the fluctuations, the finite beam sizes, and a spatial-temporal description of the phenomena. It was our opinion that such an approach might be feasible with the use of high-speed computers. Accordingly, we have written programs for the solution of the system of partial differential equations describing the propagation of light beams through fluids, for the case where thermal effects are dominant. Our calculations have been restricted to the cases showing cylindrical symmetry. In our formulation there are six dependent variables--the amplitude and phase of the electromagnetic field, the temperature and density of the fluid, and its radial and axial velocity components--and three independent variables, r, z, and t. Detailed analysis shows that the solution of the associated system of difference equations is possible if $c\Delta t < k_{\perp}(\Delta R)$, where c is the speed of light, $k_{\perp}$ is the wave number of the beam, and Δt and Δr are the mesh sizes. This relation shows that the step size in time is limited by the scale of transverse variation, and in conjunction with economic factors, limits the amount of time that the beam propagation can be followed. We have chosen, therefore, to investigate the propagation of beams of unrealistically higher power densities so that important disturbances of the beam will be produced during the time interval that we can study. The objective of the program, to gather more information on the development of beam distortions, can be met even though experiments will be performed at lower power densities. For example, if one could show that the distortions produced by the instabilities become time independent at long times, or do not, evidently a result of considerable significance bearing upon the propagation of beams

of physically realizable power densities would be achieved. Similarly, if the distortion induced on the beam was relatively mild because of saturation of the instability, or failed to develop as rapidly as predicted by the linearized instability analyses, the results would have important practical significance.

We have employed several transformations of the variables to make the equations more stable against truncation errors, and have developed several differencing schemes. At low beam powers, where there is not enough heating produced to appreciably distort the fluid, the computer solution of the difference equations does agree with expectations based upon analytic solutions of the equations of wave propagation. The result is significant in that it indicates we have succeeded in eliminating many spurious mathematical instabilities which could ruin our results. The achievement is not trivial because previously there appeared to be no practical method which enabled the evaluation of the convergence of a difference scheme as complicated as the one used for this system of equations. As the power density in the beam is raised, the density fluctuations become more pronounced, as does the distortion of the beam. The front half of the beam propagates without appreciable distortion, because the air has not had sufficient time to move and thereby produce density variations. However, the severity of the distortion grows as one proceeds toward the trailing edge of the beam, which connects with the result of the linearized instability analysis indicating that the disturbance propagates in the same direction of the beam, but with a speed equal to 1/2 c. As the beam propagates the degree of distortion grows, and, in addition, a sequence of additional pulses arise at the back boundary of the medium. Certainly this latter phenomenon is spurious, and in trying to devise methods to eliminate it we were led into a much more detailed study of the validity of differencing schemes. The standard discussion of the solution of a system of difference equations, which correspond to some system of partial differential equations, concentrates on the concept of the stability

of the differencing scheme, following an idea proposed by Von Neumann. In our problem this idea and the associated body of information concerning integration techniques are not very helpful, because our problem is known to possess instabilities. The physics produces the instabilities, and thus if we were to find a differencing scheme which was stable in the ordinary sense, we would have eliminated the essential development that we seek to analyze. In addition, the application of the standard techniques for determining convergence is unsuitable for our problem because of its complexity. For these reasons we have initiated a study of differencing schemes employing another concept, which we call "utility" in order to avoid confusion with the usual concept of "stability".

The concept of "utility" is basically very simple. A differencing scheme is "useful" if one can show that the solutions of the difference equations are sufficiently accurate approximations to the solutions of the partial differential equations over the domain of interest. Such an integration technique may not be stable, according to the Von Neuman definition of "stability", and thus may not be convergent either. This lack of stability and convergence does not cause alarm, because we can estimate the accuracy. The best analogy would be an asymptotic series expansion for a function, which certainly does not converge to the function, yet which can be a highly satisfactory description of the function over the domain of interest.

We have succeeded in developing a sufficient condition for the "utility" of differencing schemes, and have applied it to our specific problem. With its aid, we feel confident that our results have an important claim to significance. Unfortunately, we can find no evidence that the instabilities originally found by Brueckner and Jorna do not grow to be of dominant importance after a time equivalent to that indicated by their analysis. Briefly, we were surprised to find that the distortion of the beam did not develop as rapidly as one would expect upon utilizing their formula for the instability growth rate. But the fact that large distortions

develop an order of magnitude more slowly is attributable to the constraint that disturbances can be followed only if they have a transverse wavelength greater than the radial mesh size. In our case, the growth rates for instabilities with sufficiently small transverse wave number are smaller than those with maximum growth rate by an order of magnitude, thus resolving the issue.

In conclusion, our computer studies have yielded some qualitative insight into the development of distortions in high intensity beam propagation, and reinforce the suggestion that short wavelength instabilities may be of great importance in propagation phenomena.

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1.2.2 Quantum Electronic Investigation of Cross-Relaxation in Rare-Earth Crystals

NGR-05-018-044, National Aeronautics and Space Administration

L. G. DeShazer, T. S. LaFrance, M. M. Mann and D. K. Rice

Knowledge of relaxation processes in laser media is currently of great importance in understanding the interaction of radiation with optically pumped media. We are studying relaxation effects in laser amplifiers, and have concentrated our examination on neodymium crystals as the laser medium. This work is directed towards development of models for the operative relaxation mechanisms, and determination of rate equations for the spectral flux and spectral inversion density.

During this semiannual period we investigated rare-earth sesquioxide crystals, which are receiving increasingly more attention as laser media. Nd in Gd_2O_3 is a good laser host and good crystals of this material have been obtained by us recently. The difficulty in the past has been in obtaining good single crystals, but as with all crystal growth problems, the difficulty can be overcome. The absorption and fluorescence spec of Eu^{3+} in Gd_2O_3 single crystals were investigated at $4^{o}K$.[1] This work evaluated the gadolinium oxide crystal giving definite conclusions on the site and crystal symmetry, supplementing the previous x-ray data. Eu^{3+} ions occupy three nonequivalent sites of C_s symmetry extending previous crystallographic investigations. Unambiguous polarization of the absorption spectra allowed this determination. $Eu:Gd_2O_3$ is not so much of interest as a laser material but as a crystal which would help elucidate the nonradiative relaxation processes in oxides. The three nonequivalent rare-earth ions in the monoclinic sesquioxide will be an excellent source of information on cross-relaxation phenomena in oxide crystals. For instance by exciting the ions at one site and observing effects on the ions at the other sites, nonradiative processes can be studied. Such results

will be very helpful in the analyses of cross-relaxation in rare-earth glass lasers.[2,3]

Also during this period, an investigation of local fields at the site of active ions was initiated. It was theoretically demonstrated[4] that the local field at the site of atomic sources in uniaxial dielectric crystals can be determined from measurements of the spatial distribution of magnetic dipole radiation. Such local field measurements have been made[5] using the purely magnetic dipole fluorescence ($^5D_0 \rightarrow {}^7F_1$) of trivalent europium ions in single crystals of yttrium vanadate and rare-earth ethyl-sulfate. Intensities of the axial and transverse spectra in conjunction with the measured macroscopic optical indicatrix yield direct experimental values of the microscopic local field parameters g_0 and g_1. In the future these experimental results will be compared to previous theoretical interpretations.

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1.2.3 Experimental Studies in Nonlinear Optics

AF-AFOSR-69-1622A, Joint Services Electronics Program

L. G. DeShazer, L. Huff and G. L. McAllister

This experimental program is investigating nonlinear effects in the propagation of light in organic liquids. The main emphasis in this program is on nonlinear phenomena associated with the finite transverse extent of the driving optical beam.

We have investigated shaping of the time contour of intense light pulses propagating through several materials having nonlinear refractive indices.[1,2] This effect, which occurs for peak powers below the level required to form trapped light filaments with the material, is a consequence of the dynamical self-focusing of intense optical beams. Previous measurements of optical self-focusing phenomena have relied upon determination of the input power threshold for the onset of stimulated inelastic scattering. By observing the pulse shaping the nonlinear response of the medium can be constructed. Our measurements are independent of filament formation mechanisms and can be compared directly with numerical solutions of the nonlinear wave equation thought to describe self-focusing.[3]

The probe beam for the experiment is the output of a ruby laser operating in a single longitudinal and transverse mode. This single mode giant pulse ruby laser is of unprecedented quality. Its construction was made possible by a computer analysis of the laser operation which showed that the transverse intensity profile is transient and does not conform precisely to any steady-state transverse mode.[4] It also indicated how the laser parameters should be adjusted to achieve profiles close in appearance to the familiar Fox-Li modes. Good agreement between observed and predicted transverse structure was obtained for a variety of laser parameters. Such attention to the mode structure of the laser is dictated by the extreme sensitivity of the phenomena we are investigating to the transverse variation of the intensity.

The nonlinear medium is in the far field of the laser such that the input intensity profile is nearly Gaussian. The time shape of the input axial intensity is observed by splitting part of the input into a 40-ns optical delay path. The delayed pulse is directed onto a biplanar photodiode and displayed on the same oscilloscope behind the 0.07-mm aperture at the cell exit. A plot of the output intensity versus input intensity can be constructed from these two pulses. This curve is then compared to the computer solution of the simplified nonlinear wave equation. The experimental data fit the theoretically predicted curves quite closely, supporting the self-focusing theory used.[2,3]

A comprehensive theoretical treatment of saturated absorption was accomplished during this semiannual period.[5-9] An expression for the transmission as a function of incident radiant flux density was derived for an energy level model including excited state absorption. This expression was found to be a general result applicable to any model with two transitions absorbing the laser radiation under steady-state conditions. The variation of transmission with incident flux density was measured and fitted to this expression for cryptocyanine in methanol[5] and the amylose-iodine-iodide complex[7], as examples. Also, a numerical analysis of time-dependent saturation phenomena was made for optically thick absorbers, and results were presented using model parameters appropriate to chloraluminum phthalocyanine in pyridine. Observation of the temporal shaping of the laser pulse transmitted by the cryptocyanine solution was made and fitted to the time-dependent computer solution.

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1.2.4 Optical Experiments with Laser Sources

DAHC-04-69 C-0003, U.S. Army Research Office

AF-AFOSR-69-1622, Joint Services Electronics Program

W. L. Faust

Work as described in the following paragraphs is proceeding actively along three distinct lines at this point: a large, Q-switched,

tunable CO_2 laser for use in a resonance experiment; a very large far-infrared laser for study of dielectric response of simple crystals near lattice resonances; and an experiment to look for light scattering from local modes of impurity in GaP.

I. CO_2 Laser Resonances Experiment

The central item of equipment for this work is a large CO_2 laser which employs a circular diffraction grating, spinning about its normal, to achieve Q-switched operation on a single vibrational/rotational line of our choice. As early as twelve months ago we had an operating laser which produced useful power on all the reasonably strong lines. However, for purposes of a resonance experiment which we wished to perform (on the local mode in CaF_2: H), we needed some of the weaker lines, which barely ran. Also, there was some difficulty in really isolating one rotational line.

We tried a number of "improvements", particularly elimination of all Brewster windows (not successful), water cooling, three different gratings, different mirror radii. But still the operation of the laser was not fully satisfactory. More recently we have succeeded in driving the laser with pulsed discharge excitation, using a gated triode pass tube. This is somewhat difficult, because of the high voltage and rather vicious I-V characteristic for a tube with a large partial pressure of CO_2; also our discharge columns are quite long (two end-to-end, 76" and 89" long). The recent development of an 8 kV, 100 watt triode (with a BeO envelope) has made such operation practicable. To switch this pass tube, we pulse the grid and also change the value of the cathode bias resistor; the latter

is accomplished by a simple transistor circuit. With such pulsed excitation we obtain peak powers of ~20 kw on strong lines, vs. 10 kw for cw excitation. And the weaker lines which we need are doing well also, probably a few kw. To solve the problem of single line isolation we have acquired new gratings blazed at 37° rather than at 20°; other users report good results with these gratings. We consider this laser essentially ready for our resonance work in CaF_2: H.

We have in final stages of construction a second CO_2 laser of similar design except that it will not Q-switch. We expect to operate it in a quasi-cw mode with a pulsed discharge; like the first laser, it will be tunable over vibrational/rotational lines. The Q switched laser will be used to look for saturation (already seen, actually, with the sample at room temperature!) and multiple-quantum transitions with nearly resonant intermediate states. The two lasers together will be used to look for induced absorption associated with stepwise excitation.

The last piece of equipment needed for this work is the cryogenic optical system to allow optical transmission, etc., measurements on our CaF_2: H sample at the necessary temperatures of 20°K to 100°K. Shopwork is in progress, but we expect some inevitable trial-and-error delays on this matter.

In the interim we have been working with the Q-switched laser itself, studying the behavior of the optical output pulse as a function of the delay time between termination of the gas discharge and Q-switching. We have written a minor publication[1] describing the operation of the laser and the following time dependence effects observed with it:

1) Optical pulse energy vs. duration of excitation pulse;
2) Optical pulse energy vs. delay time (defined above) for lines from J = 4 to J = 42 for P and R branches of the $00^0 1 - 10^0 0$ and $00^0 1 - 02^0 0$ vibrational transitions;
3) The Q switched pulse is of greater duration when it is

delayed than when it is allowed to occur within the excitation pulse--unexplained observation.

4) The effects of varying partial pressures of N_2, He, and H_2 were studied as a function of the delay time.

II. Far-Infrared Laser Work

We have begun detailed design of a large (30 ft.) far-infrared laser, to be built in new space in Seaver Hall. We are assembling cw and pulsed power supplies for gas excitation, a vacuum-gas supply has been built, and we have infrared as well as visible detection equipment for this program. This laser will be used for infrared laser development work and for studies of dielectric properties of crystalline solids near reststrahl resonances.

III. Light Scattering

We have been able to observe Raman scattering from a doped GaP crystal, with a ruby laser source and with photographic detection. We observe intense ordinary first-order-scattering lines, previously known second-order structure (both characteristic of pure GaP), and also one or two frequencies which may be new. We will soon be able to employ photoelectric detection, which should improve our signal/noise ratio. The theoretical problem then is to interpret any frequencies which we may be able to associate (experimentally) with impurities.

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1.2.5 Coherent Optical Devices

AF-AFOSR-69-1622A, Joint Services Electronics Program

W. H. Steier, J. R. Campbell, R. Basu

I. Introduction

This work concerns the development and study of devices for the control and modulation of coherent energy in the visible and infrared wavelength regions. The devices and techniques currently under study are described below.

II. Frequency Shifter Using Lithium Niobate

A. Construction of Frequency Shifter

The basis for the frequency shifter is a single-crystal lithium niobate rod of square cross section, with light propagating along the c-axis. Modulating voltages are applied in quadrature to opposing pairs of electrodes on the crystal. The resulting rotating field inside the crystal produces the effect of a rotating birefringent plate.

Chromium-and-gold electrodes were vacuum-deposited on three sides of a 1 mm x 1 mm x 20 mm crystal. The uncoated side was fastened to a copper heat sink, which also serves as a fourth electrode and an acoustic damper. The bond was made with a thin layer of silver-filled epoxy having large thermal and electrical conductivities. Modulating voltages are applied to the electrodes by means of fine gold wires.

The frequency shifter is to be driven by a power oscillator operating in the 50-to-100 MHz range. To maximize the power delivered to the crystal, an impedance-transformer circuit was built to match the 50-ohm output impedance of the oscillator into that of the crystal. The crystal impedance consists of a capacitive reactance of the order of 10 picofarads, and a parallel resistance. The resistance depends on the loss tangent of the crystal, which has been found to vary from one sample to another. The impedance transformer consists of a pair of inductively

coupled, tuned circuits. The turns ratio of the small air-core inductors is chosen on the basis of the crystal-to-oscillator resistance ratio. Variable capacitors in the primary and secondary circuits are used to "tune out" the input and output reactances.

B. Tests of Lithium Niobate Crystals

A laboratory set-up was assembled for preliminary tests of crystal performance. A single-frequency helium-neon laser is used as the source. The laser beam is passed through a spatial filter (to remove higher-order transverse modes) and a pair of lenses which reduces the beam diameter to about 0.2 mm as it passes through the crystal. A quarter-wave plate converts the linearly polarized beam to circular polarization before it enters the crystal. A Glan-Thompson polarizing prism beyond the crystal converts changes in phase retardation (e.g., as produced by an electric field in the crystal) into changes in intensity. A photomultiplier tube is used to measure intensity.

The relative intensity of the output beam is given by

$$I = 1 + \sin 2\alpha \sin \Gamma$$

where α is the angle between the polarizer and a transverse axis of the crystal, and Γ is the phase retardation imposed by the crystal. The phase retardation is proportional to the product of voltage applied across the crystal, and the appropriate electro-optic coefficient, r_{22}.

To measure the d.c. (static) response of the crystal, the angle α is set at 45° and various d.c. voltages are applied to a pair of opposing electrodes. As indicated by the expression above, the variation of intensity with voltage will be sinusoidal. The change in voltage from minimum to maximum intensity is the half-wave voltage of the crystal, from which the static value of the r_{22} coefficient can be determined. To assess the high-frequency response of the crystal, a sinusoidal voltage $V \cos \omega t$ at the frequency ω of interest (e.g., 60 MHz) is applied. Substitution into the above expression (again setting α at 45°) shows that the intensity will now

have components varying at the frequency of the applied voltage and its odd multiples:

$$I = 1 + 2J_1(k\pi) \cos \omega t - 2J_3(k\pi) \cos 3\omega t + \cdots$$

Here, J_n is the n^{th} order Bessel function and k is the ratio of V to the (high-frequency) half-wave voltage. Qualitative observations of the intensity modulation are made by displaying the photomultiplier output on an oscilloscope. Quantitative measurement of the high-frequency r_{22} is made by comparing the first and second terms in the above series expression.

Tests have been made on two lithium niobate crystals. The first is mounted on a heat sink (as described above), and must be operated at about 170°F to relieve strain incurred during the mounting process. The second is unmounted. Both crystals exhibit good static interference figures, and d.c. values of r_{22} in good agreement with the published value. Tests at 60 MHz have indicated values of r_{22} much smaller than expected, although this may be a fault in the instrumentation. A more definitive method for measuring the high-frequency r_{22} will be implemented. This method involves heterodyning two laser beams, one of which has been modulated by the crystal. Comparison of carrier and sideband amplitudes in this way is less subject to instrumental uncertainties, particularly in photodetector efficiency.

III. Hi-Accuracy Optical Phase Measurements

The optical phase measuring set has been described in earlier reports. The accuracy of the measurements has been found to be greatly affected by electrical pickup from the room. The rotation frequency of the wave plate (57 Hz) gives a frequency shift (114 Hz) which is close to the 120 Hz room pickup. An electronic filter has been built which is very effective in removing all the low frequency noise from the output due to vibrations. The bandwidth of the filter cannot be made narrow enough to discriminate between the 114 Hz and 120 Hz.

This pickup causes a $\pm 10^{\circ}$ jitter in the phase measurements and limits the accuracy. Some preliminary phase measurements have been made with the set to verify the principle of operation. To increase the accuracy the plate rotation frequency must be increased which will entail a considerable rebuilding of the system.

IV. Parametric Oscillator Stability Studies

Some preliminary calculations have been made on the design of an optical parametric oscillator. The oscillator, when completed, will be used for the study of methods to improve the output frequency and amplitude stability.

The parameters chosen for the oscillator to be built are as follows:

a. Pump laser - Q switch Nd-YAG at 1.065μ or frequency doubled to 0.53μ.

b. Output frequency range 1.5 - 1.8 μ or 2.0 - 2.4μ.

c. Non-linear material - $LiNbO_3$.

Using published data on the birefringence and the variation of the indices with temperature, the tuning curves shown in Fig. 1 and 2 have been completed. The pump is assumed polarized as an extra-ordinary wave and the signal and idler as ordinary waves as is usually done in $LiNbO_3$. The angle θ gives the direction of propagation through the crystal and is measured from the y axis of the crystal in the x-y plane.

The tuning curves, for a fixed crystal temperature and a fixed direction of propagation in the crystal (θ), give the signal and idler wavelengths for a pump wavelength of either 1.065 μ or 0.532 μ. The signal and idler wavelengths are determined by the frequency conservation and phase match conditions

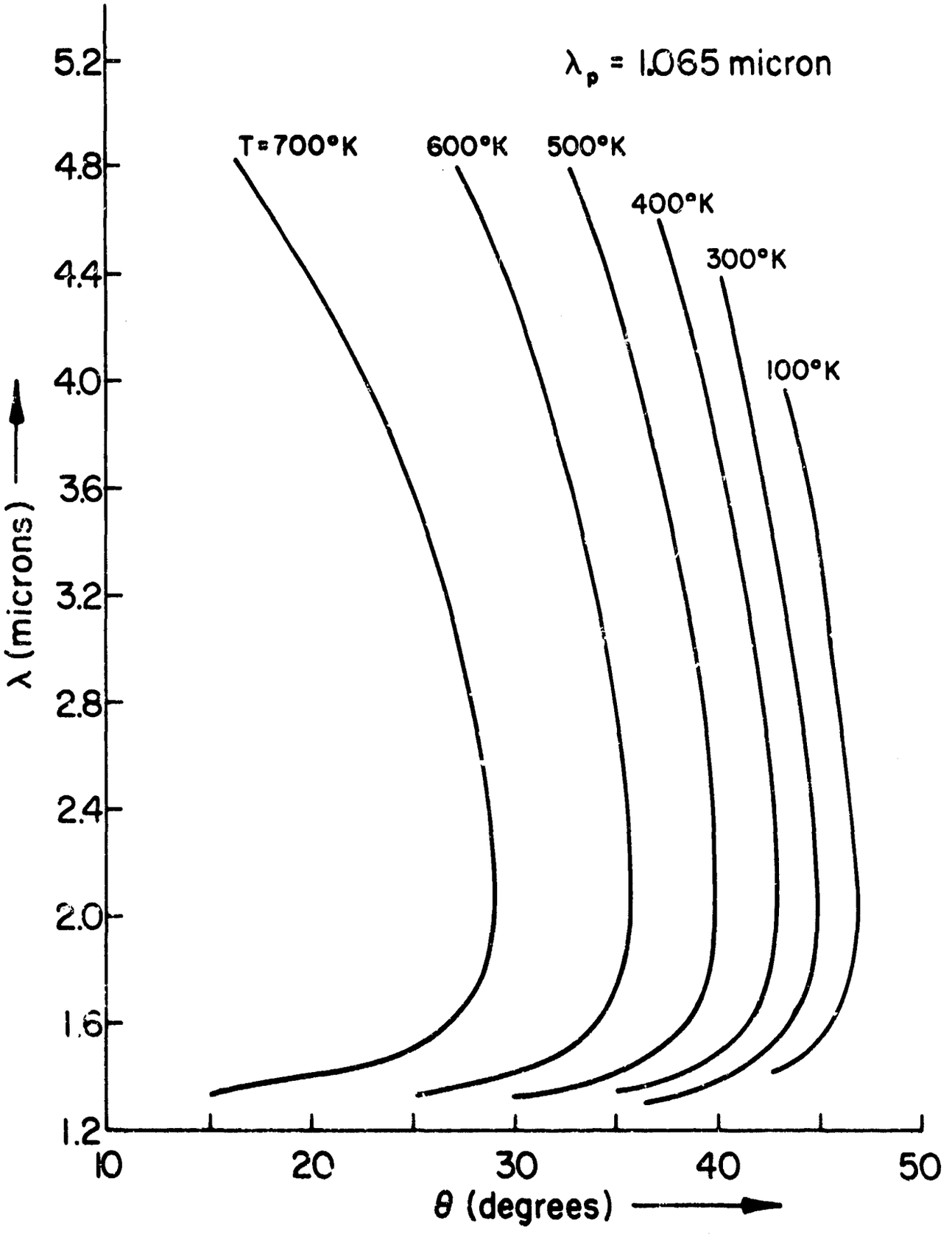

Figure 1. Parametric oscillator tuning curves for λ_p = 1.065u. Angle θ measured from y axis of $LiNbO_3$.

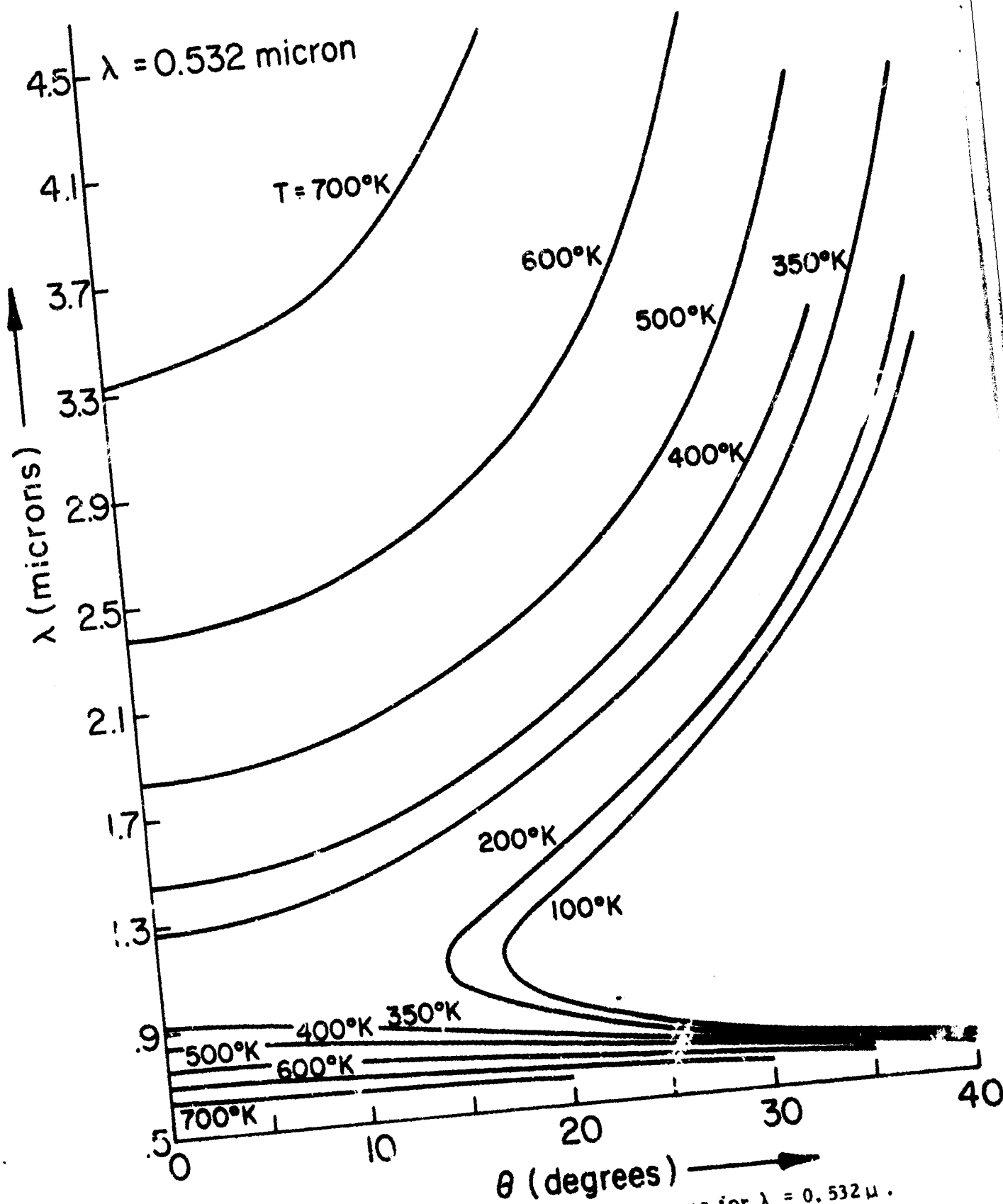

Figure 2. Parametric oscillator tuning curves for $\lambda_p = 0.532\,\mu$. Angle θ measured from y axis of $LiNbO_3$.

$$w_{pump} = w_{idler} + w_{signal}$$

$$k_{pump} = k_{idler} + k_{signal}$$

From these curves the tuning of the signal frequency can be found as the crystal temperature is changed or the crystal is rotated relative to the pump laser. For example, with a pump at 0.532 μ, a crystal at 500°K, the output can be tuned from 2.0 μ to 2.4 μ by rotating the crystal from $\theta = 11.5^{\circ}$ to $\theta = 21^{\circ}$.

1.2.6 Mixing of Internal Modes of Different Molecular Symmetry in $LiIO_3$

GP 7804, GP 15019, National Science Foundation

W. Otaguro, C. A. Arguello, S.P.S. Porto

Polarization and frequency dependence on phonon propagating directions in single crystal $LiIO_3$ were made. They showed that as the phonon propagation direction is changed, there is a continuous frequency and polarization variation with propagation direction which implies a mixing of phonon symmetries of the internal modes of the IO_3^- ion in the crystal.

It is well known that phonons which are both infrared and Raman active can have direction dependent phonon frequency and polarization. Such a phenomenon has been described for simple wurtzite type crystals[1] and quartz[2]. We would like to report such a direction dependent mixing for the case of the "molecular" crystal $LiIO_3$ which can only be understood as a direction dependent mixing of the ν_1 (symmetrical stretch) and ν_3 (asymmetrical stretch) internal modes of the IO_3^- ion.

Crystalline $LiIO_3$ belongs to the P63 (C_6^6) space group with two molecules per unit cell[3]. Group theory predicts optical phonons belonging to the following irreducible representations: $4A + 5B + 4E_1 + 5E_2$. A complete infrared and Raman analysis of those modes will be forthcoming[4].

The A and E_1 symmetry phonons are both Raman and infrared active with the A phonon polarization in the z direction (parallel to the C_6 axis) and with the E_1 phonon polarization in the (xy) plane. The E_2 phonons are only Raman active, and the B phonons both Raman and infrared inactive. The frequency of the internal modes of the IO_3^- ion obtained from IO_3^- ion solutions are[5]: symmetrical stretch $\nu_1 = 779\ cm^{-1}$, asymmetric stretch $\nu_3 = 826\ cm^{-1}$ while the symmetrical and asymmetrical bending modes ν_2 and ν_4 occur at $390\ cm^{-1}$ and $330\ cm^{-1}$. When the IO_3^- ions are in the $LiIO_3$ crystal, the factor group analysis results in an A and a B mode corresponding to the ν_1 symmetrical in phase and out of phase stretches of the IO_3^- ion and an E_1 and E_2 mode corresponding to the in phase and out of phase ν_3 asymmetric internal stretches of the IO_3^- ion. Since both the A and E_1 modes are infrared and Raman active, they will be split by the long range electrostatic forces into transverse and longitudinal optic modes. Performing the usual Raman scattering experiments using different geometries combined with polarized infrared reflectivity, these modes were observed: $A(TO) = 784\ cm^{-1}$, $A(LO) = 810\ cm^{-1}$, $E_1(TO) = 762\ cm^{-1}$, and $E_1(LO) = 838\ cm^{-1}$. From this data we see that the A_{TO-LO} long range electrostatic splitting is $26\ cm^{-1}$, the E_1 TO-LO electrostatic splitting is $76\ cm^{-1}$, the A_{TO}-E_{1TO} anisotropy splitting is $22\ cm^{-1}$ and the A_{LO}-E_{1TO} anisotropy splitting is $28\ cm^{-1}$. This crystal thus seems to be an intermediate case between Loudon's[6] case (I) ($\omega_{LO}^{\perp} - \omega_{TO}^{\perp} \gg \omega_{TO}'' - \omega_{TO}^{\perp}$ or $\omega_{LO}'' - \omega_{LO}^{\perp}$) i.e., when the electrostatic interaction dominates over anisotropy splitting and case (II) ($\omega_{TO}'' - \omega_{TO}^{\perp}$ and $\omega_{LO}'' - \omega_{LO}^{\perp} \gg \omega_{LO}^{\perp} - \omega_{TO}^{\perp}$ or $\omega_{LO}'' - \omega_{TO}''$), where anisotropy splitting dominates over the long range electrostatic field.

When propagating the phonon in the xz plane and measuring the (yy), A polarizability tensor component, and the (zy), E_1 polarizability tensor component, we observe that in the 762 - 784 cm^{-1} and 810 - 838 cm^{-1} regions of the spectrum, there is always a single phonon whose frequency and polarizability tensor changes continuously while going from $\theta = 0$ ($\bar{k}$ propagating along z axis) to $\theta = 90^{\circ}$ ($\bar{k}$ propagating along x axis). The

frequency of the phonons follows the relations:

$$\omega_{LO}^2 = \omega_{A\text{-}LO}^2 \cos^2\theta + \omega_{E_1\text{-}LO}^2 \sin^2\theta$$

$$\omega_{TO}^2 + \omega_{A\text{-}TO}^2 \sin^2\theta + \omega_{E_1\text{-}TO}^2 \cos^2\theta \qquad (1)$$

where θ is the angle formed between the phonon propagation direction and the z-axis. Figure 1 shows a comparison between the experimentally measured phonon frequencies and those predicted by Eq. 1. Figure 2 shows the relative cross-section of the (yy), A polarizability tensor component, for each phonon frequency as function of the propagation direction θ. We see from Figs. 1 and 2 that a phonon propagating at an angle θ to the z-axis will have a frequency given by Eq. 1 and mixed A-E_1 symmetry. The A and E_1 intensities of this mixed phonon as a function of θ are given by

$$I_{LO} = I_{A_{LO}} \cos\theta + I_{E_1\text{-}LO} \sin\theta$$

$$I_{TO} = I_{A_{TO}} \sin\theta + I_{E_{1TO}} \cos\theta .$$

The results show that:

1) The A and E_1 modes, (although originating from different internal normal modes of the IO_3 ion) mix.

2) The phonon mechanical polarization is always either transverse or longitudinal, showing the existence of a long range macroscopic electric field which dominates over all other designations (A or E_1, internal or external of the phonons).

This result contradicts some comments about the transverse and longitudinal nature of the polarization of phonons propagating in arbitrary directions.[7,8]

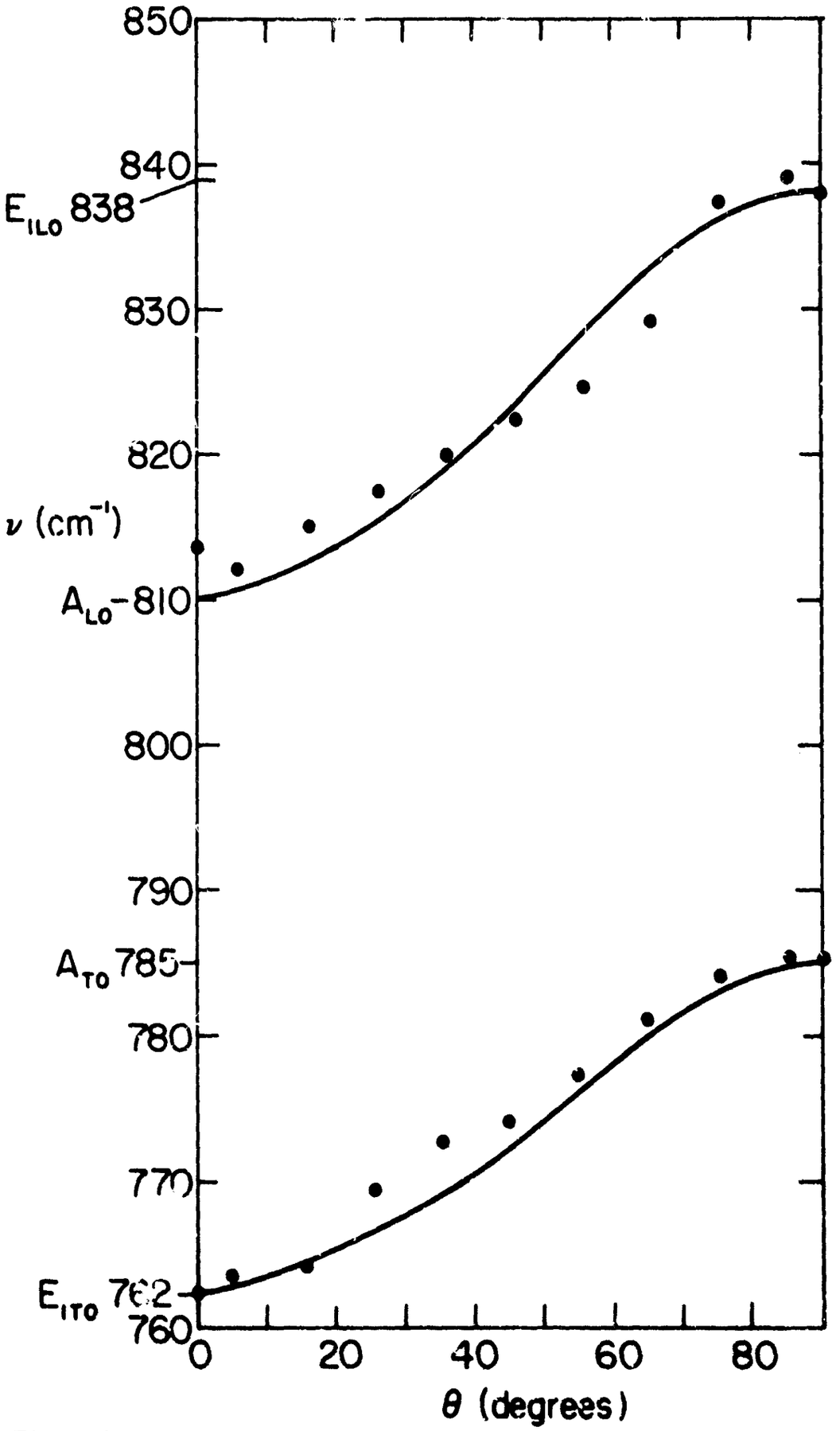

Figure 1. Variation of the frequency of the LO and TO modes of $LiIO_3$ as a function of the angle of propagation.

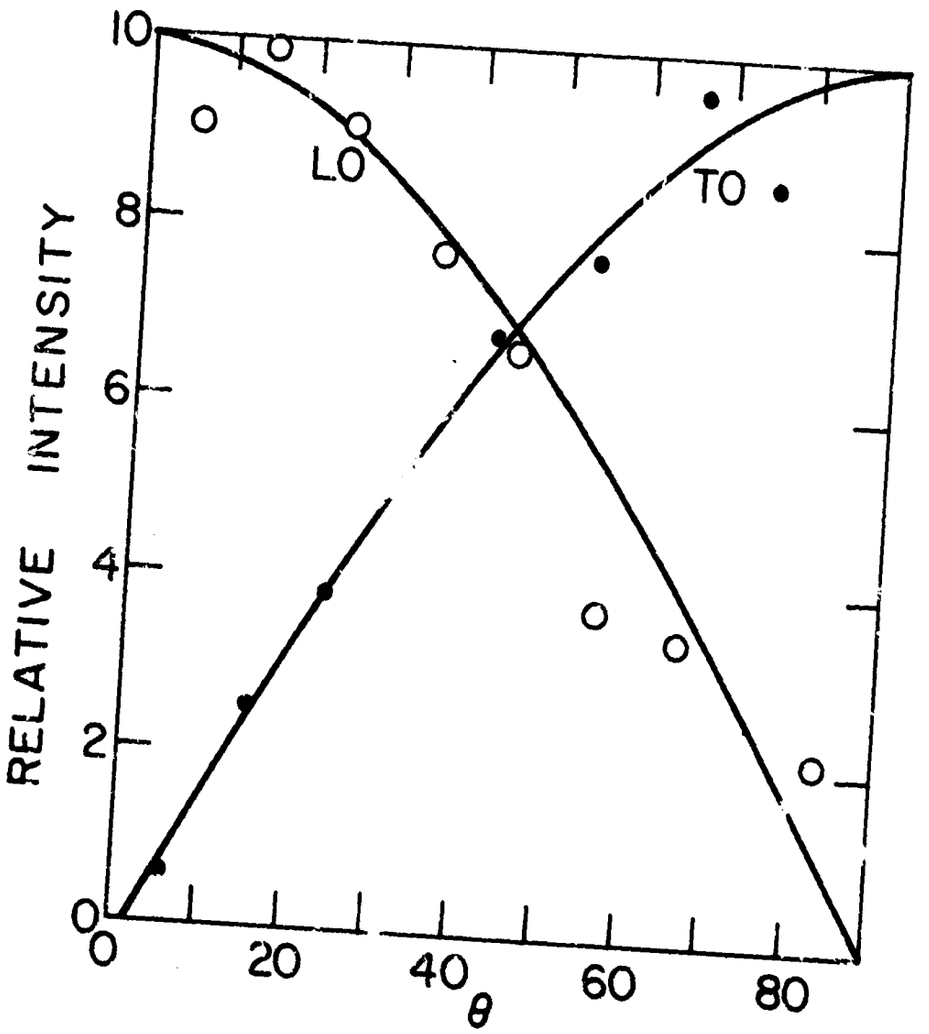

Figure 2. Relative cross section of the (yy) polarizability tensor component as a function of angle of propagation.

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1.2.7 Theory of Self Focusing of Intense Elliptically Polarized Optical Beams

AF-AFOSR-69-1622, Joint Services Electronics Program

DA-ARO-D 31-124-6920, U.S. Army Research Office (Durham)

J. Marburger, E. Dawes

The self focusing of intense optical beams in liquids whose refractive index depends upon the intensity is always accompanied by an induced birefringence. This induced birefringence causes the self focusing behavior of elliptically polarized beams to differ dramatically from that of linearly polarized beams. For example, both the orientation and the ellipticity of the polarization ellipse become sensitive functions of axial and radial distance within the medium. Previous investigations of these phenomena have been undertaken by our group in the context of the paraxial ray approximation[1]. During the past six months we have obtained numerical

solutions of the coupled partial differential equations which describe the detailed development of the optical field. These solutions confirm the existence of many of the qualitative phenomena predicted by the less sophisticated paraxial ray approach, but also yields some new results of interest.

Our solutions show that the rotation of the polarization ellipse is linear in z, the axial depth of penetration of the beam, as long as z is much less than the self focusing length. The angular velocity of the orientation angle increases as the focus is approached. At the same time however, the ellipticity also changes. This means that experiments performed in the past which infer the orientation from measurements of two linear polarization components will not give the correct result, since these components suffice to give the orientation only if the ellipticity is fixed. Another interesting feature of our solutions is the manner in which the ellipticity increases as the beam focusses itself: for low initial ellipticities (nearly circularly polarized) the ellipticity increases at first but then oscillates about the value 2. (The ellipticity is the ratio of the major to the minor axis of the polarization ellipse.) This is unexpected as simple arguments lead one to expect the ellipticity to increase without bound[2].

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1.2.8 Relaxation Oscillations in Stimulated Inelastic Light Scattering

AF-AFOSR-69-1622, Joint Services Electronics Program
DA-ARO-D 31-124-6920, U.S. Army Research Office (Durham)
J. Marburger, R. Johnson

In previous semiannual reports we have described nonstationary effects associated with the nonlinear interaction of a plane wave pump with forward and backward travelling Raman scattered waves. The behavior of the oscillations of intensity which occur was investigated as a function of the pump intensity, finite driving pulse duration, active medium length, and forward-backward Raman gain asymmetry.

During this period we extended our analysis to include coupling with an additional backward travelling wave corresponding to a stimulated Brillouin wave. We find that the nonstationary behavior of all the waves persists even with this additional coupling. A program has also been developed which allows investigation of Brillouin scattering without invoking Tang's approximation, which eliminates the rate equation for the sound wave. This approximation is only valid for pump intensities sufficiently low that the Brillouin gain length is much greater than the sound wave damping length. This inequality is easily violated in many nonlinear materials so it is of interest to have reliable solutions in this case. Preliminary solutions for a limited range of parameters show significant deviations from the predictions of the rate equations using Tang's approximation, but it is still too early to give a meaningful account of the situation.

1.2.9 Theory of Multiple-Phonon-Resonance Raman Effect in CdS

AF-AFOSR 69-1622, Joint Services Electronics Program

M. L. Williams and J. Smit

In Progress Report No. 9, Klein and Porto[1] presented Raman scattering spectra of CdS for exciting light of frequency ν_L near the fundamental absorption edge. Similar experiments have been reported by Leite, et al[2]. Raman lines with frequencies $\nu_R = \nu_L - n\nu_P$ with n up to about 10 were observed partly superimposed on a broad fluorescence. ν_P is the frequency of the longitudinal optical phonon and is about 9.10^{12}Hz. There seemed to be a correlation between the intensity of a Raman line and the intensity of the fluorescence at that frequency. We have explained these observations by a model in which resonant absorption occurs for states which are excited both electronically and vibrationally.

The effective matrix element for production of a photon of frequency $\nu_R = \nu_L - (m_g - n_g)\nu_P$ is

$$< n_L - 1, n_R + 1, m_g, g \,|H|\, n_L, n_R, n_g, g > =$$

$$h\sqrt{\nu_L \nu_R n_L (n_R + 1)} \quad N(E)\, \mu_{eg}^2(E) \sum_{n_e} \frac{<m_g|n_e><n_e|n_g>}{E - h\nu_L + (n_e - n_g)h\nu_P}\, dE$$

where the initial state has n_L and n_R photons at the frequencies ν_L and ν_R respectively and n_g phonons of frequency ν_P. N(E) is the density of electronic states. μ_{eg}^2 is the electric dipole matrix element between the electronic excited state $|e>$ and the ground state $|g>$, and n_e is the number of phonons in the intermediate state. When the electron is in the state $|e>$ the equilibrium positions of the atoms are displaced, hence phonon states $|n_e>$ for which the electron is in $|e>$ are not orthogonal to states $|m_g>$. The overlap is

$$\langle m_g | n_e \rangle = e^{-(R/2Q_o)^2/2} \sqrt{\frac{n!}{m!}} \sum_{P=0}^{n} \frac{(-1)^P}{P!} \binom{M}{n-P} (R/2Q_o)^{m-n+2P}$$

where Q_o is the R.M.S. zero point motion and R is the Fourier component of the displacements for a mode. Results were obtained for parabolic, Lorentzian, and Gaussian densities of states.

When random imperfections introduce localized electronic states, the Raman line intensity is given by the sum of the squares of the effective matrix elements for each scattering center. For the experiments being considered, the individual excited state linewidth was much less than the inhomogeneous broadening given by the density N(E). In that case the intensity of the m^{th} Stokes line is proportional to $\frac{X^{2m}}{m!} \sum_{n=0}^{m} \binom{m}{n}^2 N(h\nu_L - nh\nu_P)$. Here X^2 is the sum of quantities $(R/2Q_o)^2$ for all modes excited.

Assuming a Gaussian density of states

$$N(h\nu_L - nh\nu_P) \propto \exp\left(-\left(\frac{6-n}{1.5}\right)^2\right)$$

which fits the observed fluorescence and adjusting the parameter X^2 to 0.7, we found a reasonable fit to the data. For example for the experiment with 4579 Å excitation the relative intensities are

m =	3	4	5	6	7	8	9
I_m =	.0007	.005	.010	.012	.010	.008	.002 .

Similarly for the 5017 Å experiment predicted relative intensities:

m =	1	2	3	4
I_m =	1.12	1.05	0.46	0.18 .

Conduction band scattering also contributed to the 4579 Å first three sidebands.

It has been shown that in the limit of large phonon quantum

number the square of the effective matrix element given here yields exactly the classical intensities of sidebands produced by a frequency modulator.

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1.3 MAGNETISM

1.3.1 Investigation of Vibronic Spectra of Rare Earth Ions in Fluorite Lattices

AF-AFOSR 69-1622A, Joint Services Electronics Program

J. P. Hurrell

We have analyzed both the shape (frequency dependence) and the relative intensities of the vibronic spectra of divalent samarium ions in both BaF_2 and SrF_2 (fluorite lattices); these results have also been applied to the fluorescence of divalent europium in SrF_2. The purpose of this investigation has been to choose a model which will accurately reproduce the experimental characteristics of simple vibronic spectra. The success of the calculation depended upon choosing a relatively ideal situation where the analysis could be completely accomplished without recourse to unknown parameters.

The phonon dispersion curves of BaF_2 were measured by neutron spectroscopy and accurately reproduced by a shell model calculation. Consequently, we had a good knowledge of the phonon excitations of the pure crystal. The crystal is highly ionic and the constituent ions are only weakly polarizable. The ionic polarizabilities deduced from the shell model closely approximate the free ion values of Pauling and consequently we believe that the shell model gave not only a good fit to the phonon frequencies but also yielded realistic eigenvectors for the vibrations. This is important in the analysis of the vibronic spectra because they depend critically upon both features.

Samarium was chosen as the impurity for three reasons. Both the mass and ionic radius of samarium is close to that of barium; this ensures that the impurity is only weakly perturbing the lattice phonons and a satisfactory approximation could be obtained by neglecting this perturbation altogether. This assumption was more questionable for SrF_2 though any resonance mode, incipient or otherwise, should become

apparent in the comparison between the vibronic spectra and the model calculation. Thirdly, the fluorescence terminates on several different samarium crystal field states, well resolved in frequency and possessing different symmetry characteristics. These act as a fine probe for investigating the exact nature of the coupling between the rare earth ion and the phonons.

This interaction was assumed to proceed via the electric potential set up by the phonon at the rare earth's 4f-shell. This potential was expanded in multipole moments and the interaction Hamiltonian written as a sum of products of potential multipoles with the charge distribution multipoles of the rare earth ion. By taking due account of symmetry restrictions, one parameter was required to specify the dipolar, two parameters for the quadrupolar and three parameters for the octopolar interaction. These parameters are independent of any particular phonon, in this approximation, and are analogous to the usual static crystalline field parameters. The calculation was not taken beyond third order.

The multipoles were calculated by performing exact lattice sums for a series of k-vectors specifying the phonons and using the appropriate eigenvectors to estimate the contribution of each phonon to the multipole in question. The lattice sums were performed by the Ewald method with the convergence parameter chosen as the same for all three multipoles. None of these multipoles had been previously tabulated for fluorite lattices.

A projected density of states was calculated in histogram form for each independent member of each multipole moment and then compared to the experimental curves. Estimation of the contribution of each to a given experimental curve was facilitated by the fact that each exhibits a well-defined set of peaks which characterize the component in question. By assuming that the side bands were electric dipole in character, the quadrupole terms could be eliminated and symmetry requirements imposed the following restriction: $|{}^5D_0> \rightarrow |{}^7F_0>$ (dipole T_{1u}); $|{}^5D_0> \rightarrow |{}^7F_1>$

(dipole T 1_u); $|^5D_o> \rightarrow |^7F_2, E_g>$ (dipole T 1_u, octopole T 1_u. T 2_u); $|^5D_o> \rightarrow |^7F_2, T\ 2_g>$ (dipole T 1_u, T 2_u, A 2_u). Experimentally these restrictions were well-obeyed with the exception of $|^7F_1>$. Here the difference between $|^7F_o>$ and $|^7F_1>$ could be ascribed to magnetic dipole transitions; these allowed the quadrupole terms to contribute (both E_g and T 2_g). The reason they are so important in the $|^7F_1>$ transition lies in the fact that the dominant intermediate state for this second order vibronic process must be the $|^7F_1>$ state itself. When this is also the final state, the magnetic dipole transition intensity becomes proportional to w_p instead of $w_p^3/(w_o + w_p)^2$ where w_p is the phonon frequency and $\hbar w_o$ the appropriate crystal field splitting ($\gtrsim 400\ cm^{-1}$). Consequently, towards the center of the $|^7F_1>$ vibronic ($w_p \sim 200\ cm^{-1}$), the intensity from the magnetic dipole transition is an order of magnitude larger than for the other transitions, and becomes comparable in intensity to the electric dipole contribution.

These calculations have confirmed the long-range nature of the interaction and should be compared with the interactions assumed for the related phenomena of impurity-induced infrared absorption and Raman scattering where a nearest neighbor interaction becomes a good approximation. Apart from a calculation of absolute intensities of these side bands, the analysis is complete and a full report will soon be available.

1.4 DEFECTS IN CRYSTALS

1.4.1 Defect Chemistry of CdS

GK 4056, National Science Foundation

F. A. Kroger

1.4.1.1 High Temperature Hall Effect Measurements

F. A. Kroger and G. Hershman

Measurements of the Hall effect of CdS in equilibrium with cadmium vapor at various pressures between 600 and 1000°C show the presence of doubly ionized native defects (Cd_i or V_S). The thermodynamic parameters of the defect formation reaction and the donor ionization have been determined.

1.4.1.2 Self-Diffusion in CdS

F. A. Kroger and V. Kumar

The self-diffusion coefficient of Cd in undoped CdS is found to be independent of P_{Cd}. Since the sulfur self-diffusion coefficient is much smaller, whereas the electrical conduction varies with P_{Cd}, this indicates that Cd diffuses by means of an associate $(Cd_i V_{Cd})^x$; this corresponds to ring diffusion involving two atoms. Different behavior is to be expected in doped CdS.

1.4.2 Electrochemistry of Solids

AF-AFOSR-6801405A, Air Force Office of Scientific Research

F. A. Kroger

1.4.2.1 Zirconia as an Oxygen Pump

F. A. Kroger and D. Yuan

A paper was published: J. Electrochem. Soc. 116, 594-600 (1969).

1.4.2.2 The Sodium Activity in Liquid Na-Sn Alloys

F. A. Kroger and D. Yuan

Sodium activities were measured with a cell Na | Pyrex | Na, Sn. The results were published in J. Phys. Chem. 73 (7) 2390-2392 (1969).

1.4.2.3 Pyrex Glass of Oxygen and Sulfur Electrode

F. A. Kroger and D. Yuan

Cells of the type

$$\text{Na} \mid \text{Pyrex} \mid \text{Pt}, O_2 \qquad \text{(a)}$$

$$\text{Na} \mid \text{Pyrex} \mid \text{C, S(g) or } H_2S \qquad \text{(b)}$$

$$\text{Pt}, O_2 \mid \text{Pyrex} \mid \text{Pt}, O_2 \qquad \text{(c)}$$

give emf's according to the Nernst formulae

$$E = E_o + \frac{RT}{4F} \ln p_{O_2} \qquad \text{(a)}$$

$$E = E'_o + \frac{RT}{4F} \ln p_{S_2} \qquad \text{(b)}$$

$$E = \frac{RT}{4F} \ln (p_{O_2})_r / (p_{O_2})_l \qquad \text{(c)}$$

with E_o and E'_o determined by the activity of Na_2O and Na_2S in the glass.

Polarization varies E_o by varying a_{Na_2O}, but steady state, no polarization values are re-established after some time.

1.4.2.4 Polarization Studies on AgCl

F. A. Kroger and Y. Van der Meulen

Both hole and electron conduction have been studied using Wagner's polarization method. Values for the product of the concentrations of electrons and holes $np = K_i$ are compared with values calculated on the basis of optical band gap data. Hole mobilities are determined using published hole absorption data. A discrepancy is attributed to the presence of self-trapped holes; the latter causes the optical absorption, while the conduction involves free holes.

A paper has been accepted for publication by J. Electrochem. Soc.

1.4.2.5 I-V Characteristics of Zirconia Cells

a) F. A. Kroger, H. Yanagida and R. J. Brook

b) W. L. Pelzmann, R. J. Brook and F. A. Kroger

a) Cells

$$Pt, O_2 \mid ZrO_2 \mid Pt, O_2$$

were investigated, using porous Pt past electrodes. The cells give non-ohmic characteristics. Two regions are to be distinguished:

I. low voltage: $I \propto p_{O_2}^{1/2}$

The rate limiting step is diffusion of O^- through the Pt.

II. high voltage: I independent of p_{O_2}

The rate limiting step is the transfer of O, adsorbed and ionized at the free electronically conducting surface of Pt into vac[illegible] the zirconia ZrO_2.

A paper has been [illegible]ted to J. Electrochem. Soc.

b) The effect of the structure of the Pt cathodes is investigated, comparing Pt cathodes of varying porosity with non-porous Pt films of varying thickness (made by sputtering or from pressure contacted Pt foil). Oxygen diffusion through the Pt is suppressed in the thicker films, and the free surface mechanism II is absent with non-porous electrodes. These show instead $I \propto p_{O_2}^{-1/4}$ due to electronic conduction (which is accompanied by F center formation).

1.4.3 Defect Chemistry of Al_2O_3

N 00014-67-A-0269-0007, Office of Naval Research

F. A. Kroger

1.4.3.1 High-temperature Conduction of Al_2O_3

R. J. Brook, F. A. Kroger and J. Lee

Work on the determination of transference numbers and the measurement of electrical conduction of pure and doped single crystals of Al_2O_3 is continued. Cobalt increases the conductivity; Ti has no effect. Presently, our efforts are focussed on the extension of the measurements to the range 1000 - 2000°C where equilibrium with the atmosphere may be established. A new high-temperature furnace has been put in operation but is still giving difficulties.

1.4.3.2 Valency Variation of Transition Elements in Al_2O_3

F. A. Kroger and J. Chang

A cooling device to make possible low temperature absorption measurements has been put in operation. Spin resonance equipment is being designed.

1.4.4 Defect Chemistry of SiO_2

Supported by TRW

T. G. Mills and F. A. Kroger

Conductivity measurements of 5000 Å thick films of SiO_2 formed by thermal or steam oxidation of pure and doped Si have been carried out as f(T).

The dopant has an effect on the properties of the SiO_2. It is attempted to find the contributions from electronic and ionic dark conductivity and space-charge limited electronic currents. Emf measurements of cells Si | SiO_2 | Si, Ge indicate that the SiO_2 has an ionic transference number of $t_i \approx 0.15$.

It has proved possible to obtain free films of SiO_2 by removal of Si from Si/SiO_2 by etching. It is the intention to use these in cells Pt, O_2 | SiO_2 | Pt, O_2 for measurements of the conductivity and the t_i. The effect of p_{O_2} and p_{H_2O} on the conductivity will be investigated. Attempts are being made to determine the thermoelectric power.

1.5 METALS, ALLOYS, INSULATORS AND LOW TEMPERATURE PHYSICS

1.5.1 Fundamental Studies of Explosive Shock Loading by Transmission Electron Microscopy

NGR-05-018-044, National Aeronautics and Space Administration
AF-AFOSR-69-1622, Joint Services Electronics Program

L. E. Murr, H. R. Vydyanath and W. N. Lin

The purpose of this research program is the basic study of very high pressure shock deformation on the structure and properties of metals and alloys. The approach utilizes electron transmission microscopy techniques to observe the residual shock deformation substructures.

Investigations of particle statistics for unshocked TD-Ni (2.3% ThO_2) and TD-NiCr (2% ThO_2) have been completed. Typical results for each material following a 1200°C anneal for 2 hours are shown in Figs. 1 and 2. It is noted that the mean particle diameter for the ThO_2 dispersoid is approximately 330 Å in the TD-Ni and 170 Å in the TD-NiCr. We would expect, therefore, that the shock response of each microstructure might be distinctly affected because of the mean free path difference, and its effect on the propagation of matrix glide dislocations.

Sheet samples of Inconel 600 alloy (76% Ni, 16% Cr, 7% Fe) and Chromel-A alloy (78% Ni, 20% Cr) were simultaneously shock loaded in sandwich assemblies[1] at pressures of 80, 180, 240 and 460 Kilobars. The residual defect structures in Inconel 600 and Chromel-A were characterized by planar dislocation arrays exhibiting a prominence of dislocation loops and dipoles. Deformation twins having an average width of 150 Å were observed to nucleate in the shock-loaded Inconel 600 in the pressure range 200-240 Kb when considering the previous results of Murr and Foltz[2]. The critical twinning pressure for the Chromel-A was roughly 240 Kb. Figure 3 illustrates the comparative microstructures for the

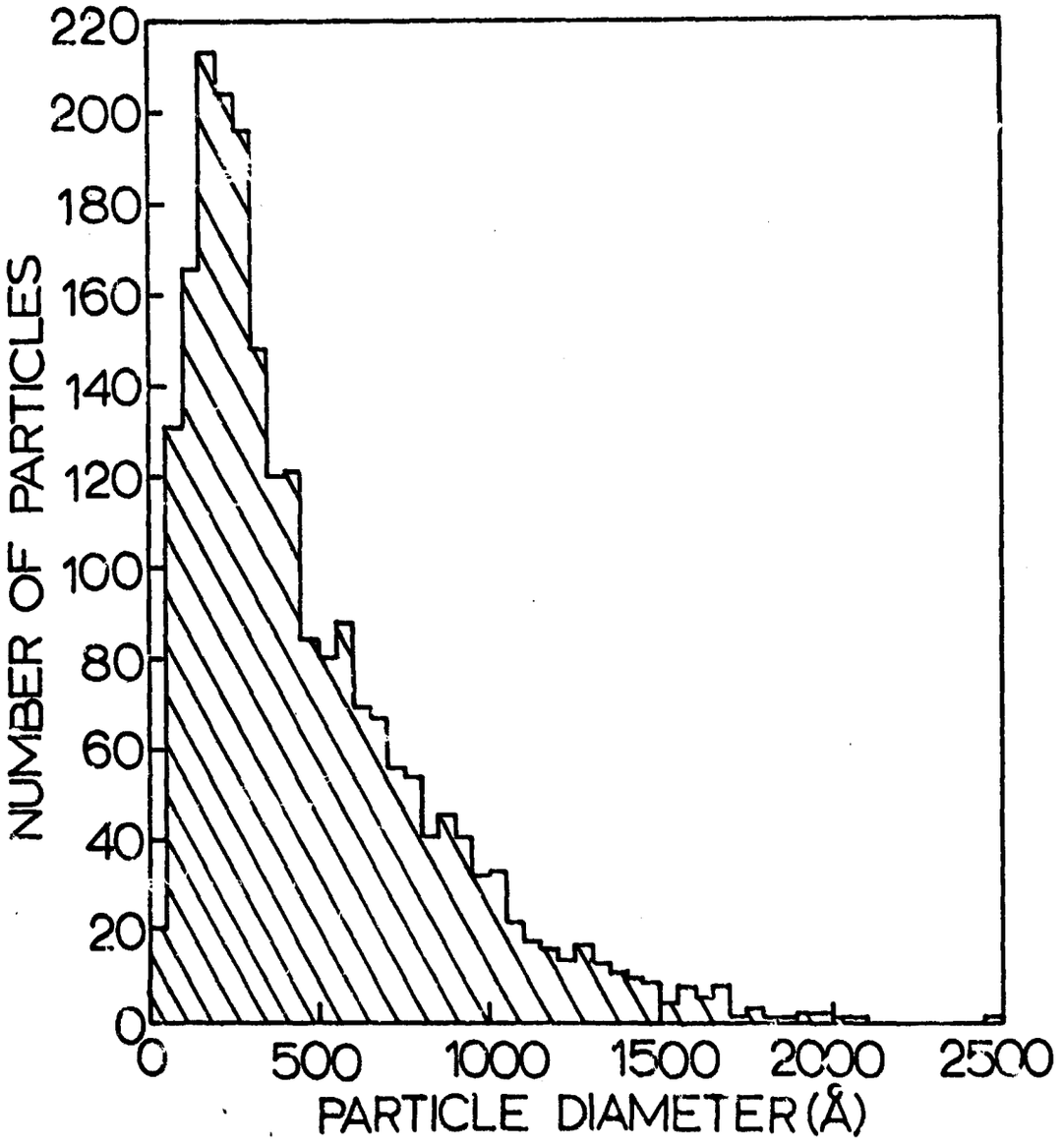

Fig. 1 Thoria Particle Size Distribution in TD-Ni Following 2 Hour Vacuum Anneal at 1200°C.

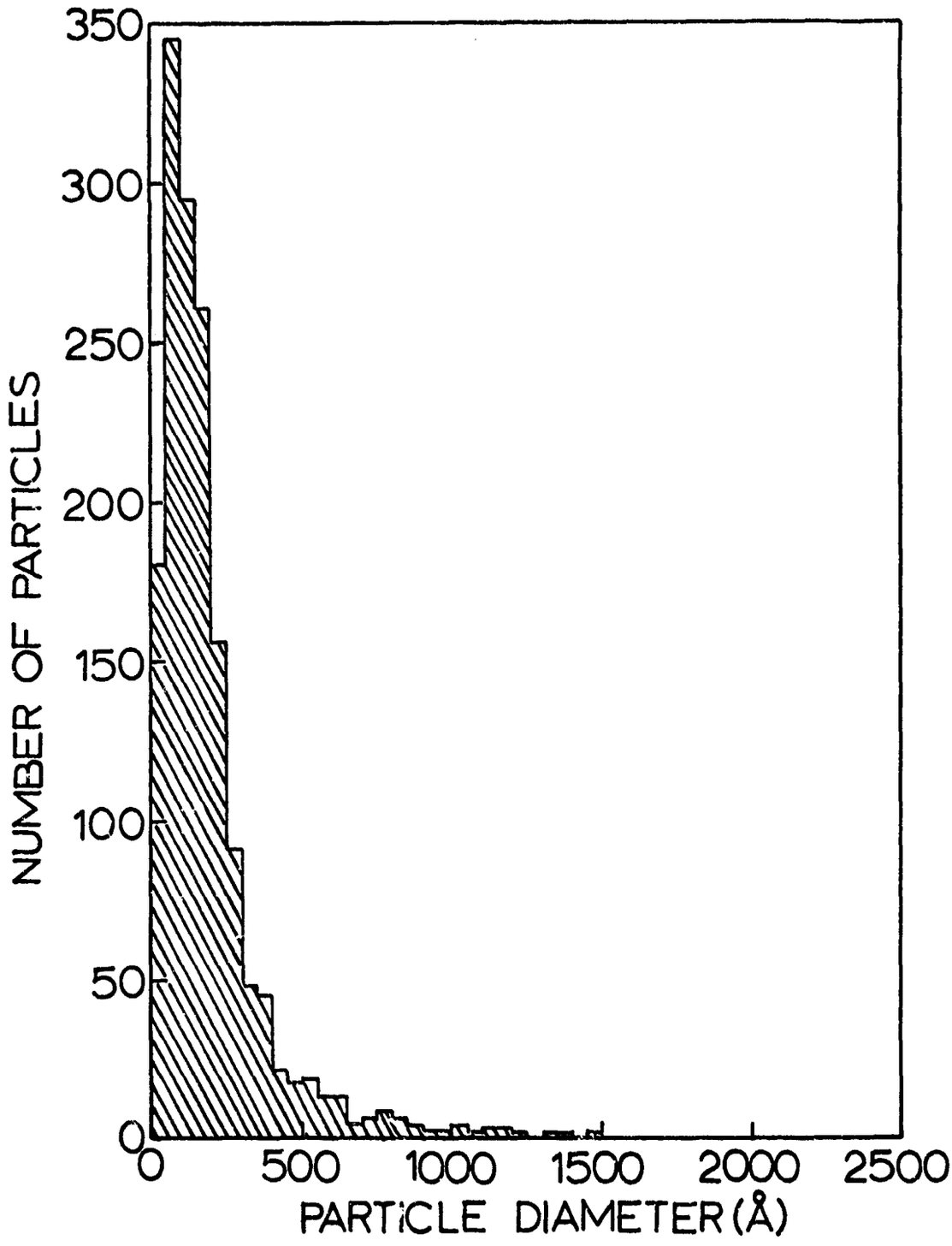

Fig. 2 Thoria Particle Size Distribution in TD-NiCr Following 2 Hour Vacuum Anneal at 1200°C.

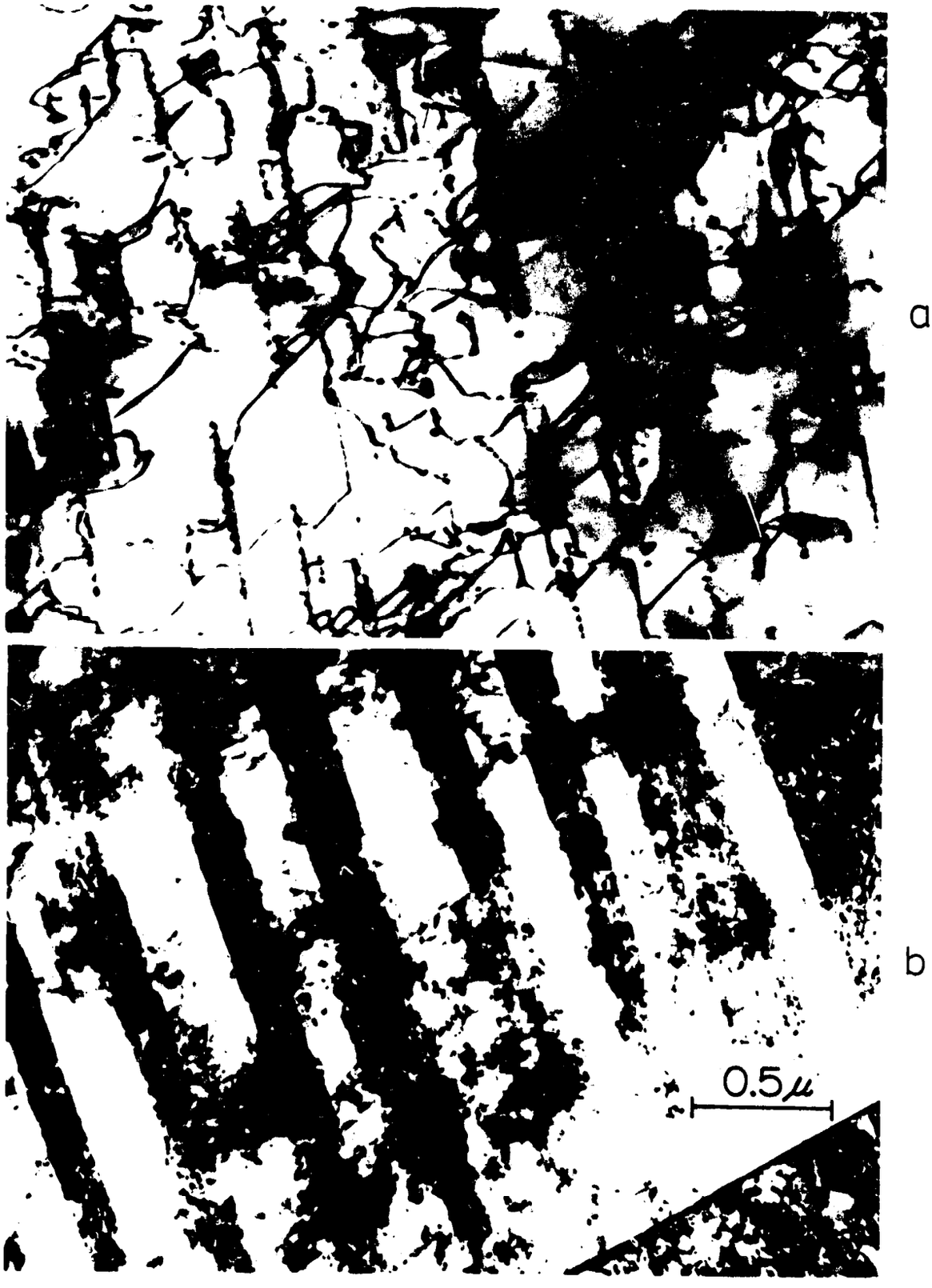

Fig. 3 Bright-field transmission electron micrographs of Shock-Loaded Chromel-A. (a) Dislocation substructure following 80 Kbar shock loading. (b) Twin structures following 460 Kbar shock loading.

Chromel-A shock loaded at 80 and 460 Kbars.

Twin volume densities at 240 Kb were observed to be 14 and 5 percent for the Inconel and Chromel, respectively; at 460 Kb, the corresponding volume density of twinned material was 24 and 18 percent, respectively.

A detailed comparison of the microstructures revealed that prismatic dislocations in the Inconel and Chromel are the most likely sources of deformation microtwins for shock pressures above the critical twinning pressure. This evidence suggests that a pole mechanism[3] for twin formation is increasingly prominent in shock deformed materials of high stacking-fault energy (>25 ergs/cm^2), and that twinning in shock-loaden nickel[1] is probably completely dependent upon prismatic twin sources.

Figures 4 and 5 illustrate a comparison of the residual dislocation densities and microhardnesses for the shock-deformed Inconel and Chromel. It is readily observed that the majority of the residual hardening is due to a densification of the dislocation substructures.[4]

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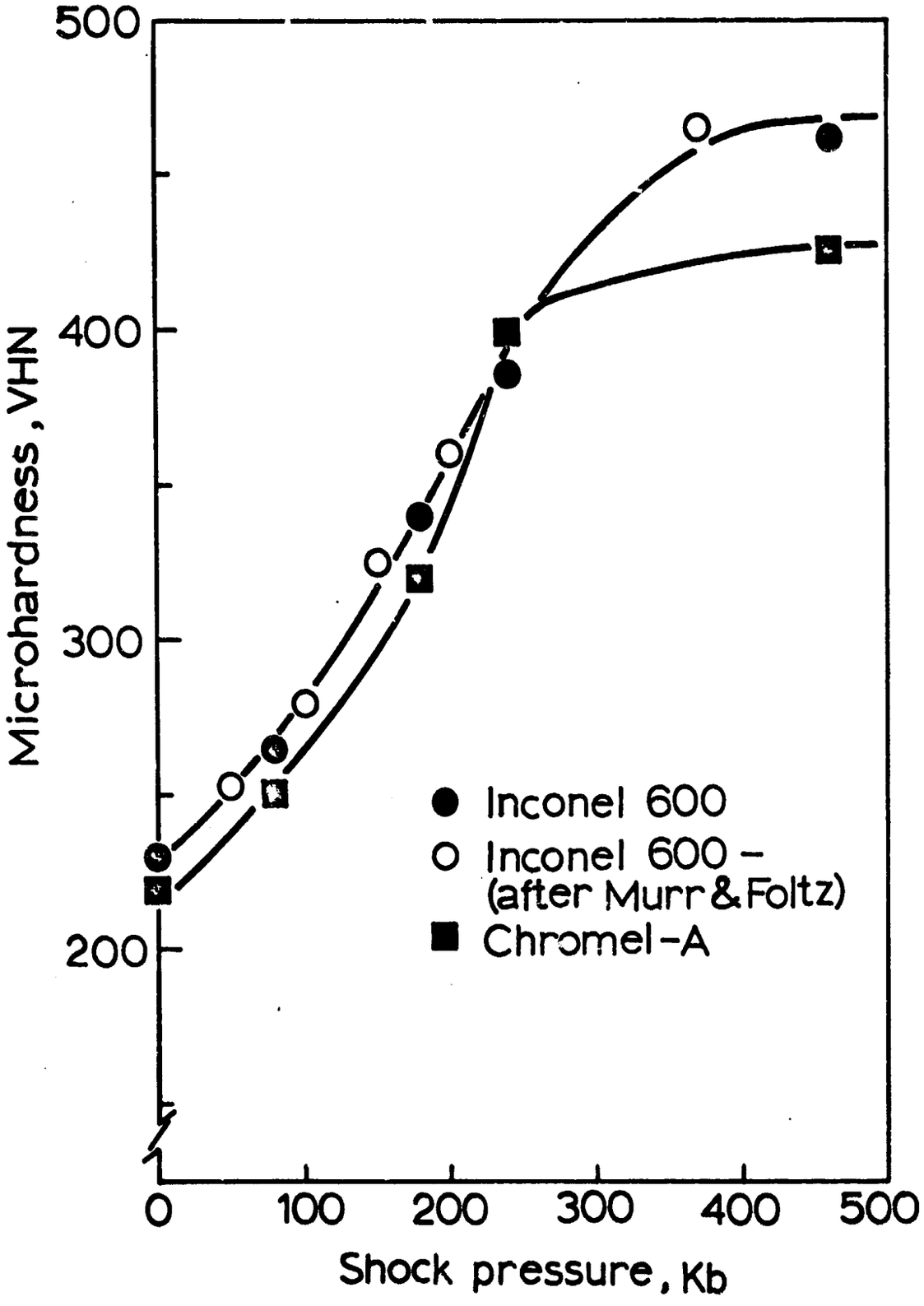

Fig. 4 Vickers microhardness versus explosive shock pressure.

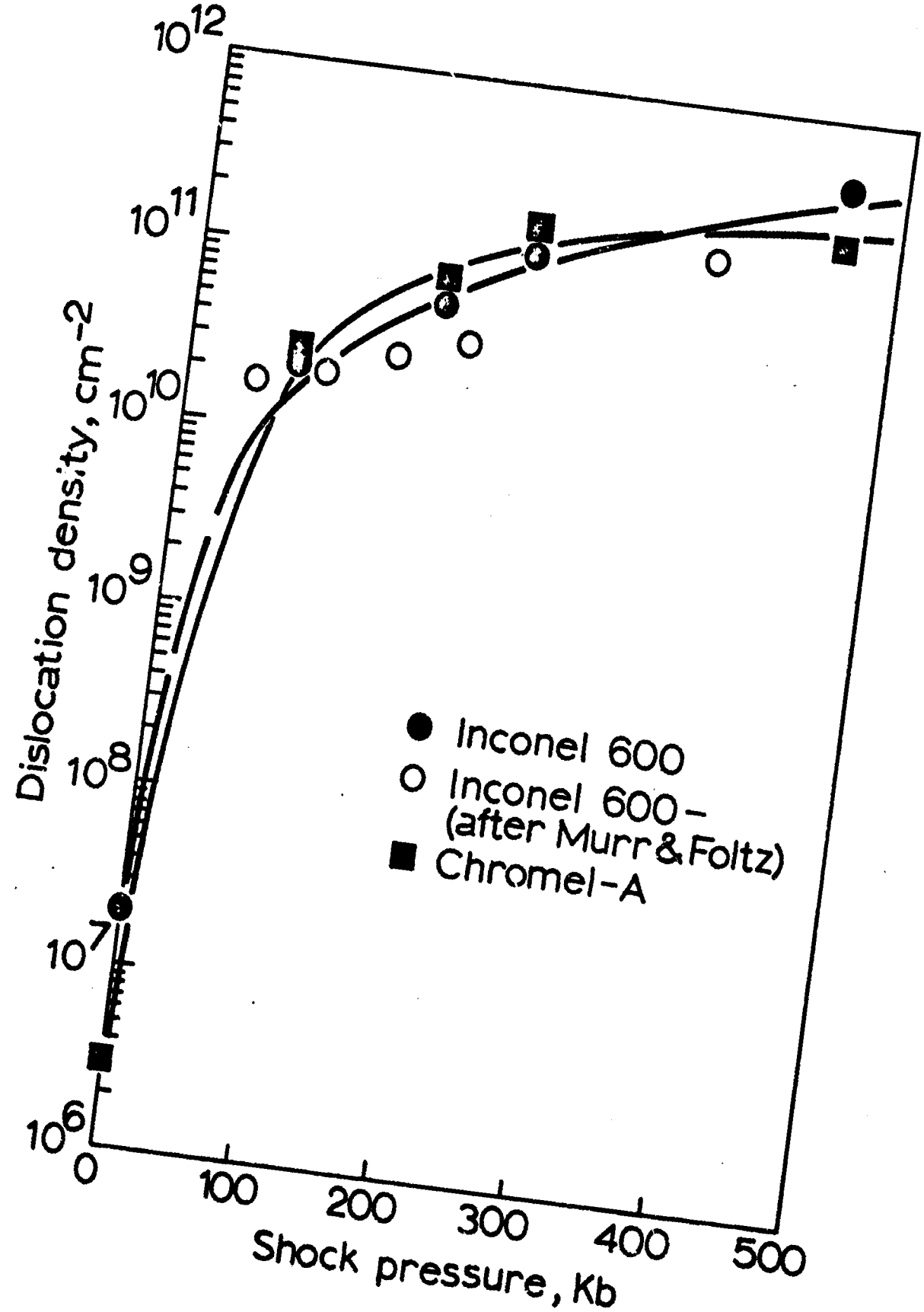

Fig. 5 Dislocation density versus explosive shock pressure.

1.5.2 Measurement of Interfacial Free Energies in Solid Metals and Alloys

N00014-67-A-0269-0010, Office of Naval Research

L. E. Murr, R. J. Horylev and W. N. Lin

The purpose of this research program is the characterization of interfacial free energy and structure in metals and alloys by transmission electron microscopy.

Several significant accomplishments have been attained within the present report period. These will be elaborated upon categorically as follows:

A. Configurational Equilibrium at Twin-Grain Boundary Intersections in F.C.C. Metals and Alloys, and the Measurement of Relative Interfacial Torque[1]

By considering the misorientation of <110> directions between certain unique crystallographic orientations at twin-grain boundary intersections in thin metal and alloy foils, a configurational theory has been developed which is applicable in explaining the origin of intrinsic interfacial torque. This theory is shown to be applicable with an average confidence of 80% in the analysis of twin boundary-grain boundary intersection systems using electron transmission and selected-area electron diffraction microscopy techniques.

By considering equilibrium systems as shown in Fig. 1, it can be assumed that ΣM can represent a resultant or net effective torque resolved parallel to the twin boundaries; having equal magnitude but opposite sense. For the coherent twin-grain boundary intersection systems shown in Fig. 1(a)-(c), it has been shown that[1]

$$\frac{\gamma_{tb}}{\gamma_{gb}} = \frac{C_{AB} + C_{T_AB}}{2}$$

$$\frac{\Sigma M}{\gamma_{gb}} = \left| \frac{C_{AB} - C_{T_AB}}{2} \right|$$

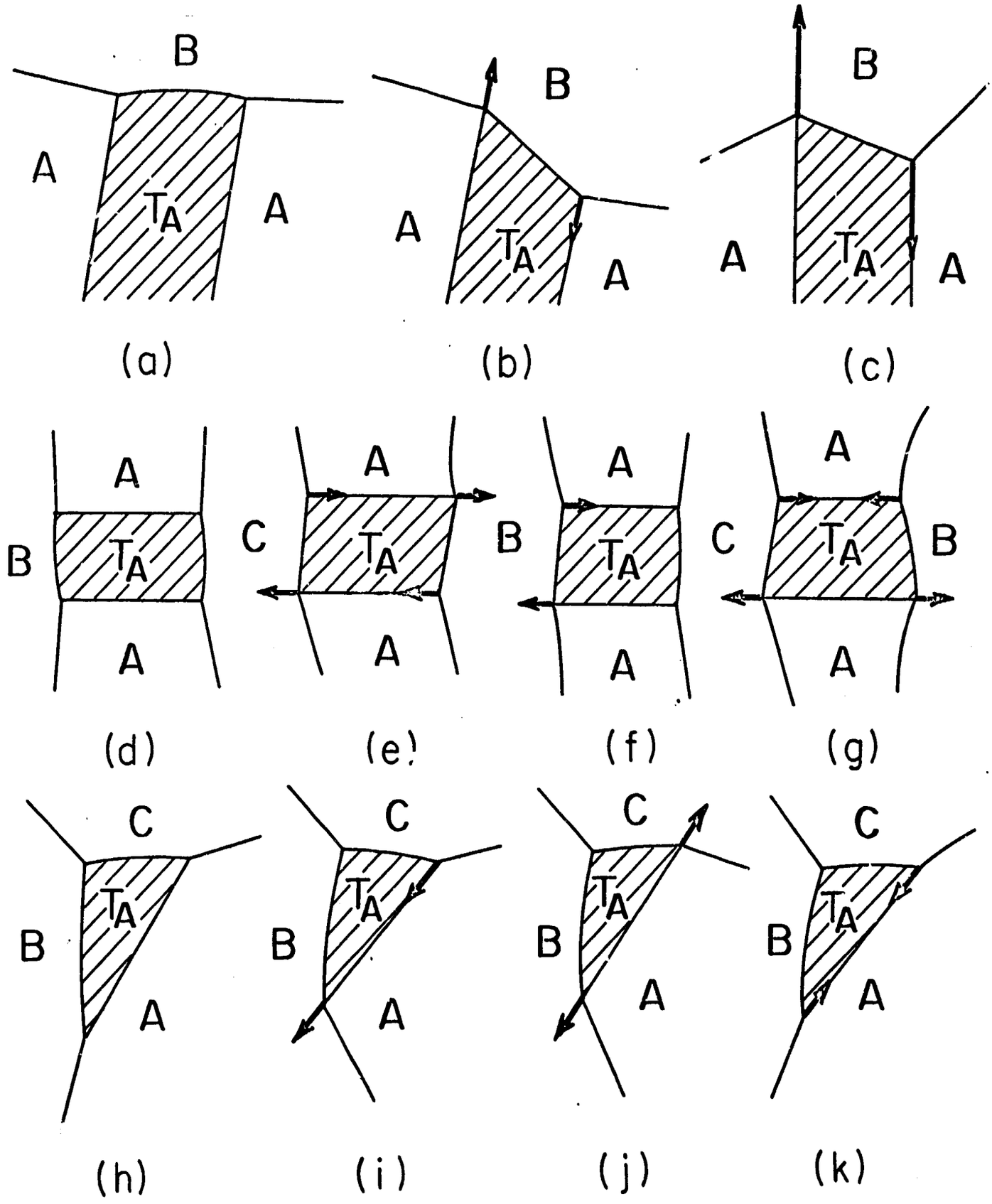

Fig. 1 Equilibrium twin-grain boundary junction configurations. The heavy arrows indicate the sense and relative magnitude of net effective torques resolved parallel to the twin boundary.

where γ_{tb} is the coherent twin boundary free energy, γ_{gb} is the grain boundary free energy, ΣM is the interfacial torque, and

$$C_{AB} = \frac{\cos \Omega_2 \cos \Omega_4 - \cos \Omega_1 \cos \Omega_3}{\cos \Omega_3 - \cos \Omega_2}$$

$$C_{T_A B} = \frac{\cos \Omega_2 \cos \Omega_4 - \cos \Omega_1 \cos \Omega_3}{\cos \Omega_1 - \cos \Omega_4}$$

where the Ω_i's are the true dihedral angles of intersection as given previously by Murr[2].

Defining intrinsic interfacial torques to arise primarily because of a change in grain boundary free energy with a variation in <110> misorientation, Θ, low-torque configurations are described by those where the relative interfacial free energy ratios which arise at the interface between grains A and B, γ_{tb}/γ_{AB}, and between the twin of grain A, T_A and grain B, $\gamma_{tb}/\gamma_{T_A B}$ (Fig. 1 (a)-(c)), are essentially equal. High torque configurations are those where geometrical ratios related to the interfacial energy ratios differ by more than 10% for specific crystallographic situations which promote a significant change in the <110> misorientation across the twin and intersecting grain interfaces. Figure 2 illustrates the typical configurations for high and low torque twin-grain boundary intersections.

The mean ratios of net effective torque to a grain boundary free energy, $\Sigma M/\gamma_{gb}$, for high-torque configurations observed in thin foils of nickel, 304 stainless steel, Inconel 600, and Cu-5 at % Al were measured as 0.0188, 0.0082, 0.0073 and 0.0091, respectively. Table 1 illustrates typically the comparative situations for high and low torque configurations similar to Fig. 2. The analysis for stainless steel in Table 1 corresponds to the images of Fig. 2.

The configurational theory has also been extended to double

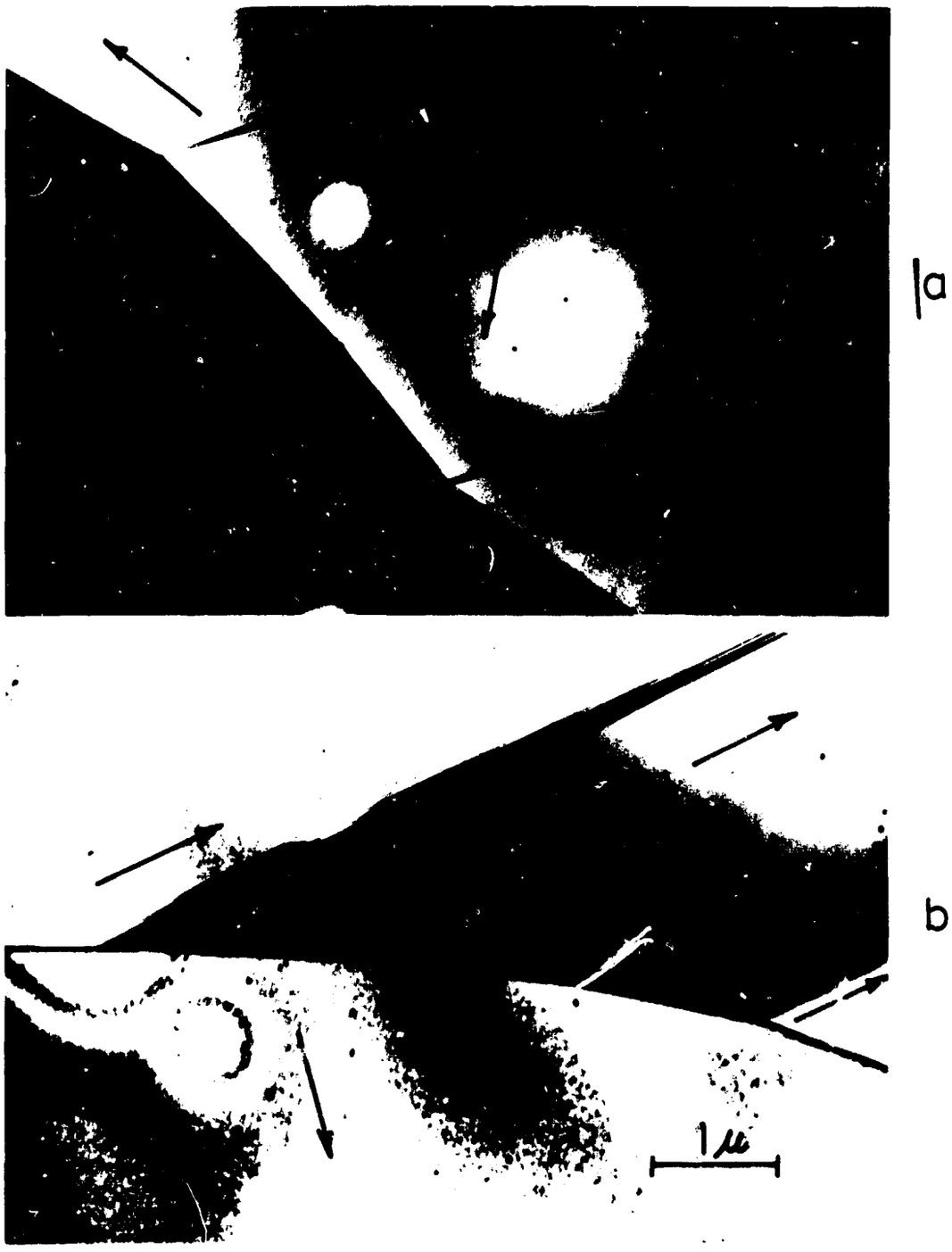

Fig. 2 Bright-field electron transmission images of twin-grain boundary intersections in 304 stainless steel. (a) High-torque configuration; (b) Low-torque configuration. Arrows indicate $[1\bar{1}0]$ directions. All grain surfaces are (110).

Table 1. Analysis of Selected Electron Transmission Images

Material	Torque Configuration	Grain Surface $(hk\ell)_A$	Grain Surface $(hk\ell)_B$	True Dihedral Angles (deg.) Ω_1	Ω_2	Ω_3	Ω_4	<110> Misorientation (deg.) Θ_{AB}	Θ_{T_AB}	C_{AB}	C_{T_AB}	γ_{tb}/γ_{gb}	$\Sigma M/\gamma_{gb}$
304 Stainless Steel	low	(110)	(110)	76.8	105.8	71.7	109.8	80	80	0.0348	0.0360	0.0354	0.0006
304 Stainless Steel	high	(110)	(110)	51.5	114.4	63.7	136.7	79	77	0.0252	0.0159	0.0205	0.0093
Nickel	low	(110)	(110)	74.7	106.5	73.6	108.2	46	46	0.0254	0.0250	0.0252	0.0002
Nickel	high	(103)	(112)	90.4	106.9	71.4	93.1	--	13	0.0298	0.3881	0.2090	0.1792
Cu-5 at % Al	low	(110)	(110)	56.8	124.8	55.2	126.3	73	73	0.0219	0.0220	0.0220	0.001
Cu-5 at % Al	high	(112)	(110)	90.8	96.7	82.5	92.3	55	--	0.0260	0.2477	0.1369	0.1109

twin-grain boundary systems (Fig. 1(d)-(g)) and the high-temperature equilibration of grain-corner twins (Fig. 1(h)-(k)).

B. Interfacial Energy and Structure in F.C.C. Metals and Alloys.

It has been shown by transmission electron microscopy that a rather obvious distinction exists for the interfacial free energies of high-angle grain boundaries, low-angle grain boundaries, and twin boundaries in fcc metals and alloys[3]. The characteristics of these differences have been analyzed and a balance of interfacial free energy argument used to calculate relative interfacial free energy ratios.

The average low-angle grain boundary free energy in nickel and 304 stainless steel was found to be 383 and 342 ergs/cm^2 respectively, corresponding to average misorientations of 1.9° and 1.7°. The coherent twin boundary free energy in nickel and stainless steel was found to be 41 and 18 ergs/cm^2 respectively, while the ratio of coherent twin boundary free energy to noncoherent twin boundary free energy was measured as 0.070, 0.090 and 0.100 in nickel, 304 stainless steel, and Cu-5 at % Al respectively. Utilizing absolute grain boundary energy measurements for nickel and 304 stainless steel also allowed the complete characterization of interfacial free energies in a metal and alloy for the first time. These results are summarized in Table 2.

Dislocation core energies have been measured for nickel and 304 stainless steel as 1.2 and 1.3 eV per atomic length of edge dislocation; representing approximately 6% of the corresponding dislocation self-energies.

It has also been shown by transmission electron microscopy that low-angle grain boundaries of the general tilt variety possess a predominantly edge dislocation structure, while high-angle grain boundaries in fcc metals and alloys possess a variable structure consisting of infrequent dislocations, steps, ledges, and a high proportion of coincident boundary-plane sections.[4]

Table 2. Relative Interfacial Free Energy Ratios and Average Interfacial Free Energies*

	Nickel	304 Stainless Steel
γ_{tb}/γ_{gb}	0.049	0.023
γ_{tb}/γ_{TB}	0.070	0.090
γ_{TB}/γ_{gb}	0.700	0.253
γ'_{gb}/γ_{gb}	0.455	0.432
γ_{gb}/F_s	0.400	0.380
γ_{SF}/γ_{tb}	7.300	1.200
Specific surface free energy, F_s	2100 ergs/cm^2	2080 ergs/cm^2
High angle grain boundary free energy, γ_{gb}	840 ergs/cm^2	790 ergs/cm^2
Low-angle grain boundary (tilt) free energy, γ'_{gb}	383 ergs/cm^2	342 ergs/cm^2
Coherent free energy, γ_{tb}	41 ergs/cm^2	18 ergs/cm^2
incoherent twin boundary free energy, γ_{TB}	588 ergs/cm^2	200 ergs/cm^2
Stacking-fault free energy (intrinsic), γ_{SF}	300 ergs/cm^2	21 ergs/cm^2

*All values except those involving γ_{SF} correspond to T = 1060°C. Values of γ_{SF} are assumed to be stabilized at room temperature.

The interfacial free energy of high-angle grain boundaries can vary from 3 to 6 times the average low-angle grain boundary free energy over a range of misorientations $10^{\circ} < \theta < 90^{\circ}$. Grain boundaries having energies between the mean value of low-angle and high-angle grain boundaries, and misorientations $2^{\circ} < \theta < 8^{\circ}$, possess a complex, transitional structure. Grain boundaries in fcc metals and allous act as sources of imperfections; specifically dislocations are emitted from steps or ledges in the grain boundaries which in many instances are coincident with the {111} planes.

A remarkable compatibility of interfacial structure and energetics has been observed, and a simple phenomenological model proposed for the observations of grain boundary structure which is essentially consistent with the experimental findings. This model envisions grain boundary formation as the result of atomic slip on {111} planes, or the analogous shuffling of other coincidence planes to produce dislocation-ledge structures.

C. A Comparison of Grain Boundary and Matrix-Crystalline Fracture in Ti-Mo Wires by Scanning Electron Microscopy

It was brought to our attention by Mr. Larry Robinson of this department that Ti-Mo elements in a sublimation pump strain annealed to form prominent crystallized segments along the axis of the wires, with grain boundaries between the segments aligned approximately normal to the wire axis. It became apparent that in light of our present results and conclusions regarding grain boundary structure and energy as outlined above in (B), that this particular feature presented a rather natural opportunity to investigate the nature of grain boundary fracture; and to compare the structure of grain boundary fracture surfaces with those associated with normal matrix fracture.

Figure 3 illustrates the physical appearance of the crystalline wires. The grain boundaries are clearly defined and there is evidence of

Fig. 3 Optical micrograph of strain annealed Ti-Mo wire segment.

grain boundary sliding. Spectrographic analysis of the wires indicated a molybdenum content ranging from 10-14%, with only 0.004% Mg as an impurity; with the balance Ti. The wires were observed to have a bcc structure characteristic of the β-isomorphous Ti-Mo phase; with a lattice parameter of 3.26 Å.

By gripping the wires firmly on either side of a grain boundary, the wire could be fractured in a brittle manner at the grain boundary, or over a portion of the boundary plane. This feature is shown in Fig. 4, which also exhibits irregular fracturing off the grain boundary plane by matrix cleavage. The cleavage planes were observed to be the {001} planes. It is noted in Fig. 4 that the grain boundary plane is completely smooth, with a complete absence of irregular surface cleavages, etc. The grain boundary plane in Fig. 4 was observed to be essentially a (111) plane. Similar observations of grain boundary fracture surface crystallographies also revealed a coincidence with the (320) plane, and several deviations from (111) of approximately 5 degrees. Because of the nature of the fracture surface at grain boundaries, the crystallographic coincidence of the fracture surfaces, it appears that the grain boundaries are essentially coincidence lattice planes as indicated in the previous transmission electron microscopy studies outlined in B.

By comparison, the fracture of the wire sections in the crystalline matrix between the grain boundaries was characterized by cleavage fracture along the {001} planes. Figure 5 is typical of the matrix-crystalline fracture surface. The irregular nature of the cleavage surfaces in comparison with the grain boundary surface (Fig. 4) attests to the generally unique-continuous crystallographic nature of the grain boundary.

In Fig. 6 is shown the typical fracture surface for polycrystalline Ti-Mo wires prepared by effectively very short anneals, which produced an average, fine grain size of 0.6 mm compared with the 2 mm single crystal segments shown in Fig. 3. The polycrystalline fracture is

Fig. 4 Scanning electron micrograph (using secondary electrons) of the fracture surface associated with a grain boundary in a crystallized Ti-Mo wire. The wire axis is essentially coincident with [111] as shown.

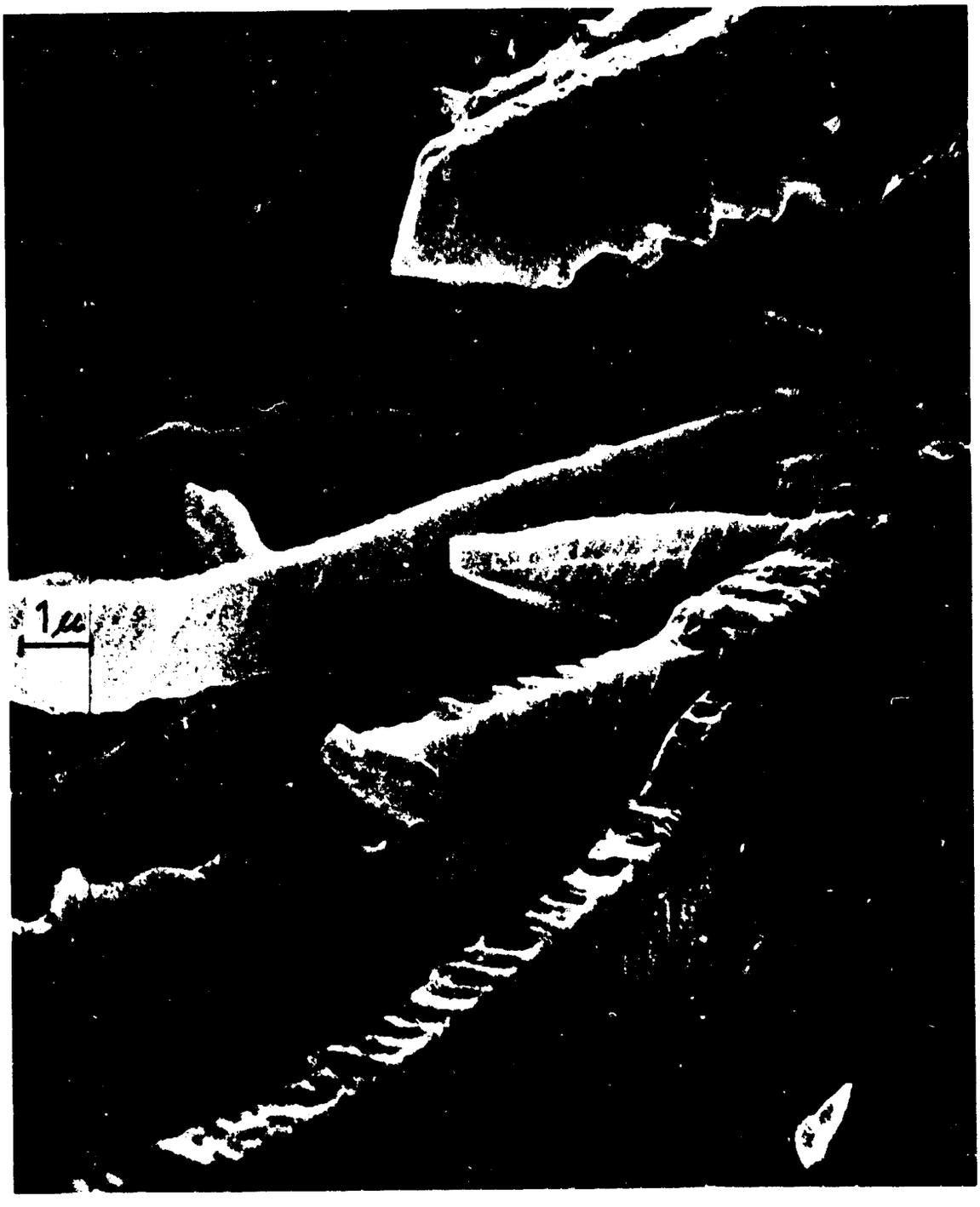

Fig. 5 Scanning electron micrograph of matrix-crystalline fracture (cleavage fracture) in a Ti-Mo wire. The cleavage surfaces are coincident with {001}.

Fig. 6 Scanning electron fractograph of fracture surface of polycrystalline Ti-Mo wire.

observed to be characterized by semi-ductile facets and small cleavage regions.

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1.5.3 The Effects of Electric and Magnetic Fields on the Nucleation, Structure, and Residual Properties of Vapor Deposited Metal Films

AT911-1)-113, Project #22, Atomic Energy Commission

L. E. Murr and H. R. Vydyanath

This study entails the simultaneous investigation of the effects of electric and magnetic fields on the nucleation mechanisms, the growth, and the terminal structure of vapor deposited films of Pd, In, Fe, Co and Gd. It is also intended to relate electrical (resistivity) and magnetic (susceptibility) property responses with the terminal film structures observed by transmission electron microscopy; and to attempt to develop a coherent understanding of how an electric or magnetic field can be used to produce possible, desired residual electronic or related physical properties in vapor deposited thin films.

During the current report period, the necessary systems for controlled evaporation were designed and constructed. These consist of

two glass ultra-high vacuum units similar to those previously described by Murr[1,2]; and a special unit for developing the necessary field variables during ultra-high vacuum vapor deposition. The special unit incorporates the earlier 1 liter chamber designs[1,2] in a similar arrangement which includes a set of polished electrodes positioned 0.5 cm below the substrate surface; capable to sustaining a potential difference of 10 Kilovolts. An electrode arrangement is also available for applying an electric field normal to the substrate; parallel to the vapor flux. This arrangement will generate an electric field parallel to the substrate surface having a gradient capable of attaining approximately 8 KV/cm. A large field coil wound of 18 gauge, heavy formvar coated copper wire, weighing 240 pounds, and containing a total of 6000 turns was designed to be positioned around the evaporation chamber to generate a magnetic field of several thousand gauss directed normal to the substrate; parallel to the main vapor flux. Figure 1 illustrates the appearance of the evaporation chamber with field coil lowered (Fig. 1(a)) and raised in normal operating position (Fig. 1(b)). We are currently calibrating the field parameters--electric and magnetic, leak detecting the vacuum systems, designing and constructing bake-out facilities; and testing the vacuum response of the individual systems.

Since it has been previously shown that evaporation variables such as residual pressure, substrate temperature, and rate of evaporation will markedly alter residual vapor grown film structure[2,3] it is necessary to completely characterize the no-field film structures. In particular, it is desirable to determine the optimum substrate temperature to insure maximum grain size and crystal perfection. Preliminary

experiments of this type are in progress at 10^{-6} torr vacuum in a commercial vacuum unit incorporating a specially designed copper substrate arrangement similar to those employed in the glass evaporation chambers, c.f. Fig. 1(a). The results for In indicated that the optimum film growth occurs at a substrate temperature of approximately 130°C. In Fig. 2 is reproduced a typical transmission electron micrograph of the residual indium film structure for vapor deposition at 130°C. The substrate material in the present experiments, and for those to be conducted in the electric field arrangements, is (001) oriented NaCl cleaved crystals. This substrate material is particularly advantageous in that the films may be easily detached for observation by transmission electron microscopy.

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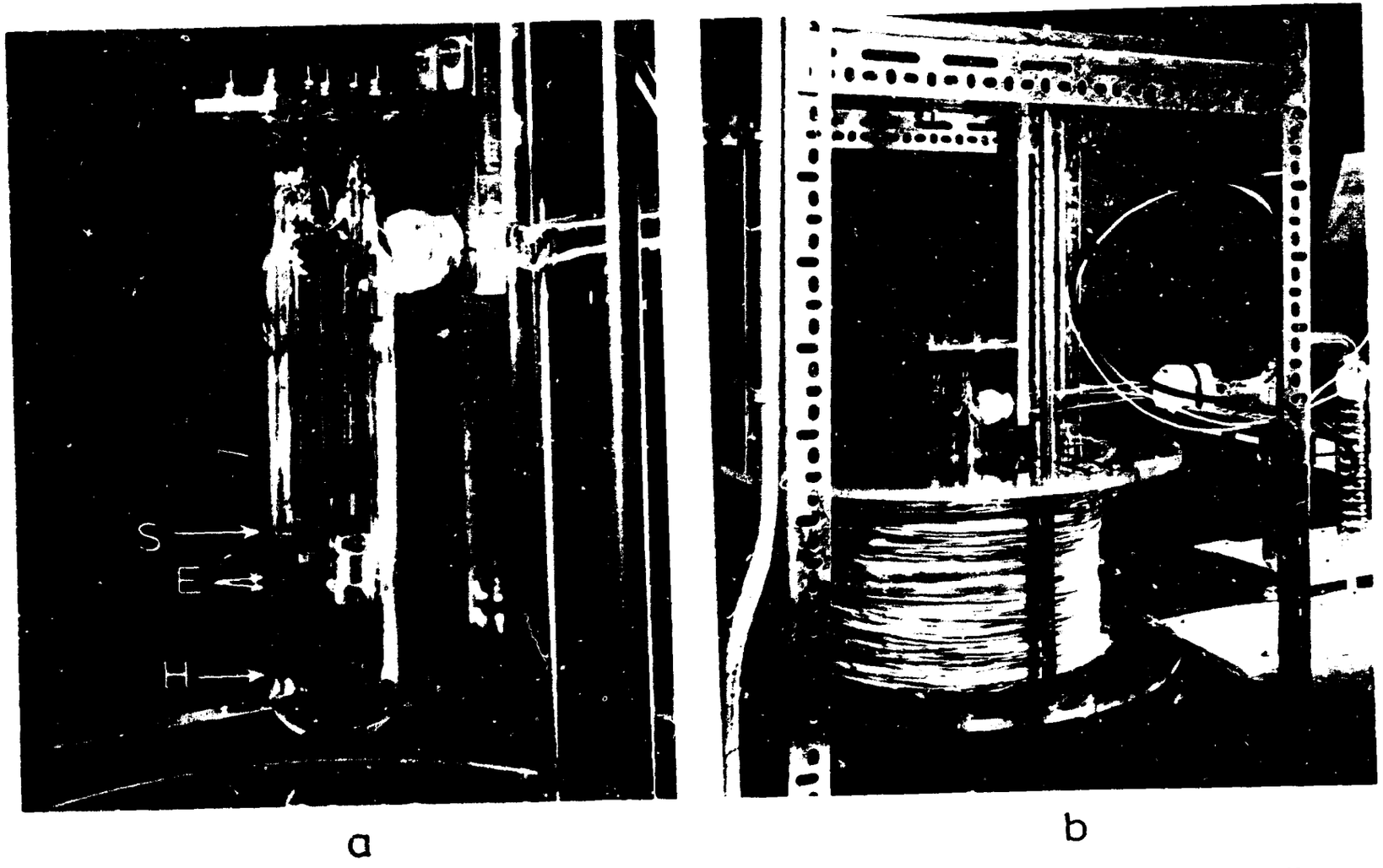

Fig. 1 Ultra-high vacuum electric-magnetic field evaporation chamber. (a) Magnetic field coil lowered to expose chamber components; S - substrate heater, E - electric field electrodes, H - source holder. (b) Field coil raised into normal operating position.

Fig. 2 Bright-field electron transmission micrograph of an indium foil area vapor deposited onto an NaCl (001) substrate at 130°C. The evaporation rate was approximately 1000 Å/sec; and the film thickness shown was approximately 1000 Å.

1.5.4 Experimental Studies of Fermi Surface Topology in Metals

AF-AFOSR-69-1622, Joint Services Electronics Program

M. H. Halloran, J. Brewer, R. Parker

This area of research is primarily concerned with the determination of Fermi surface information which is important for the improvement of the understanding of the electronic band structure of pure metals, and for a better understanding of the interactions of conduction electrons with phonons, magnons, foreign atom impurities and lattice defects. Materials of primary interest are the transition and rare earth metals, and several intermetallic compounds.

During the past six months the research has progressed in four basic areas: low field, de Haas-van Alphen (dH-vA) studies (0-28 kOe) of the Fermi surface of $AuGa_2$ using a torsion balance; high field, magnetothermal oscillation studies of $AuGa_2$ using a new adiabatic sample rotating apparatus in a superconducting solenoid, development of high purity vanadium samples using an electron beam zone refiner, and development of sample preparation techniques for low defect ultra-high purity mercury samples.

The low field dH-vA measurements in $AuGa_2$ are nearly complete. The results have verified both the original earlier results[1] and also the recently reported existence[2] of a new section of Fermi surface not detected in the earlier results. These experiments have been extended from $1.2^{\circ}K$ to at least $10^{\circ}K$ to check on possible frequency changes with temperature, but no changes were observed. Such changes would be anticipated if the tentative explanation[3,4] for the anomalous Knight shift of the Ga nucleus is correct. That explanation requires a full band at $T = 0$ to be just below the Fermi surface and to become partially depopulated as T increases. The uncertainty remains, however, since the upper limit on T for observing the dH-vA effect may be too low for

significant depopulation to have occurred. A stress apparatus to produce uniaxial strains in the sample is being constructed and will be used to depopulate the band if it exists.

The high field dH-vA measurements in $AuGa_2$ have been in progress since August. All reported data have been verified and several new features have been observed. The total Fermi surface is very complicated and the data are often too complex for analysis by hand. We have incorporated electronic filtering techniques, have completed construction of a sweep controller which provides a constant value of $\frac{d}{dt}(1/H)$, and will soon have a data processing system in use in conjunction with the new IBM 360/65 computer to facilitate the data analysis.

The electron beam zone refiner, obtained last winter for the production of high purity metal crystals, has been modified to enhance its performance and safety. Preliminary tests have been completed with some tantalum samples, and we are now beginning to purify some vanadium samples to be used for Fermi surface measurements. These vanadium samples were all spark cut from the same high purity rod, and have initial resistance ratios of approximately 25. With successful purification, they should yield sufficient data to compare with the recent results[5] on Nb and Ta.

During the past summer, extensive progress was made developing techniques for handling ultra-pure, defect free mercury crystals--particularly in regard to the attachment of leads and thermometers. We have developed a technique for spot welding leads to the sample by a capacitor discharge process while the sample is immersed in a cryogenic fluid. To attach carbon resistance thermometers, different adhesives were found to be most convenient for use at liquid N_2 (at $78^{\circ}K$) temperatures and at dry ice temperatures ($\sim 195^{\circ}K$), but bonds can be provided under both temperature environments. We are presently working on techniques to spark cut the samples.

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1.5.5 Rare Earth Metastable Solid Solutions

AF-AFOSR 69-1622A, Joint Services Electronics Program

R. Wang

Rare earth metastable solid solutions can be obtained by rapid quenching alloys from its liquid state to room temperature. The objectives of this research are to investigate:

a) limited solid solutions of non-soluble elements into rare earth metals,

b) stability ranges of the rare earth high temperature allotropes (structure b.c.c.),

c) precipitation mechanism in supersaturated alloys,

d) quench in defects in rare earth metals and alloys.

A splat cooling apparatus has been constructed so that alloys can be melted by electric induction heating and blasted into small droplets by a shock wave from high pressure helium gas[1]. Quick quenched thin foils can be directly examined by x-ray diffraction and electron microscopy.

All the rare earth high temperature allotropes are able to be retained in room temperature either from rapid cooling the pure metals or alloying with magnesium. The range of stability has been greatly extended.

Work was also concentrated on the formation of supersaturated solid solution of tin and indium to the rare earths and vice versa. Their precipitation mechanism and possible defects are under investigation.

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1.5.6 Metastable Microcrystalline and Crystalline Phases of Transition Metal Alloys

AF-AFOSR 69-1622A, Joint Services Electronics Program

R. Wang

Based upon the possible high supercooling temperatures of low melting eutectics of several transition metal systems, microcrystalline phases are able to be formed in some Ni and Zr based alloy systems[1,2]. The formation of these microcrystalline phases may be controlled by

a) the cooling rate of quenching molten alloys to room temperature, and

b) narrow range of composition near their eutectics.

The stability of the microcrystalline phases is first time investigated in ternary system. Titanium-copper-silicon alloys were prepared with Si content up to 20 atomic percent. Alloys were splat cooled from melting points to room temperature. Thin foils were examined by electron diffraction and transmission electron microscopy. The presences of the microcrystalline phases are confirmed and shown in Fig. 1. The particle sizes are estimated to be $50 \sim 200$ Å. X-ray diffraction of the thick samples indicate a new metastable crystalline phase formed in the wide range of Ti-Cu-Si composition. The metastable phase was identified to be face centered cubic. The diffraction halos of microcrystalline phase are coincided with the sharp f.c.c. lines which indicate the microcrystalline phase is actually also f.c.c. but having very small particle size due to the high cooling rate in thin sections of the sample.

Transmission electron microscopy also leads to the observation of small precipitates in the microcrystalline matrix as shown in Fig. 2.

Work is in progress to explore more microcrystalline phases in a wide range of stability. Both cooling rate and composition of the alloys are important to the formation of the microcrystalline phase. It may conclude that the formation of the microcrystalline phases in ternary

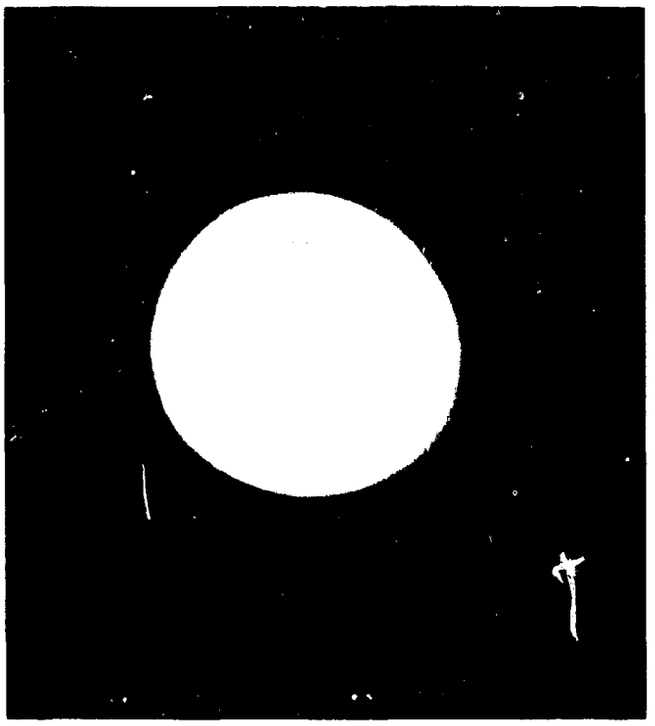

Fig. 1 Electron diffraction pattern of a thin section of Ti-Cu-Si alloy 40/40/20 atomic percentage

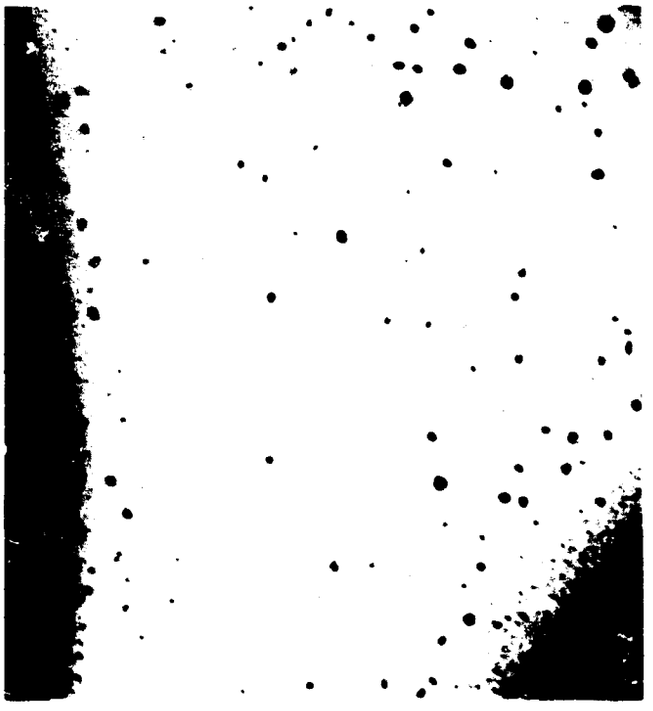

Fig. 2 Precipitates in the microcrystalline phase of Ti-Cu-Si alloy 35/55/10 atomic percentage

transition metal alloys are due to the high super-cooling temperatures.

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1.5.7 Localized Moments in Metals

GU 1559, National Science Foundation

M. D. Daybell

An atom that normally possesses a magnetic moment, such as iron or vanadium, may or may not retain that moment when it is alloyed into a normal metal, like copper or gold. Over the past two years, it has been learned that whether or not it does so depends on the temperature of the material when the measurement of its moment is carried out. Below a certain temperature T_K for each alloy, called the Kondo temperature, the moment disappears in all cases so far investigated. The variation of T_K from alloy to alloy is apparently such that $\log T_K$ is proportional to the number N of magnetic electrons in the dopant atom. This logarithmic dependence of T_K on N is reasonably well established only for iron group dopants in gold. However, the other properties of these dilute magnetic systems have nearly all been established by experiments in copper based alloys, which are now fairly well understood in many cases[1]. Unfortunately, the relative difficulty of preparing some of the copper based alloys (for example, vanadium as a dopant in copper) has resulted in a lack of data on the systematic variation of $\log T_K$ with N in these systems. A knowledge of T_K for titanium and vanadium in copper has prevented any convincing proof of the $\ln T_K$ vs. N conjecture to be obtained in any host material other than gold. We are trying to obtain such information by measuring T_K for vanadium in copper. The requisite alloys have now been prepared, and preliminary measurements are in progress.

As the properties of a single localized moment are becoming better understood, it becomes feasible to attack the problem of the interaction of one moment with another by studying the concentration dependence of the bulk properties of alloys containing local moments. These kind of measurements could eventually lead to an understanding of ferromagnetism in a large class of alloys between magnetic and non-magnetic constituents,

although there are some foreseeable metallurgical problems in even binary alloys containing more than a small percentage of magnetic component. A promising candidate for beginning this study is the system of binary alloys of small amounts of manganese in copper, where the local moment remains almost uncompensated down to quite low temperatures (T_K here is below 100 milliKelvin). As a result, moment-moment interactions are relatively strong even in very dilute concentrations of manganese, and the interaction effects are relatively easy to observe. In cooperation with Visiting Professor T. Ohtsuka, a sequence of these alloys has been prepared and its resistivity vs. temperatures is being measured.

Spin compensation of the local moments formed in transition metal based alloys is only beginning to be investigated in enough detail to establish whether they also exhibit a systematic variation of T_K with dopant spin. The molybdenum based series has had enough attention that it appears fruitful to look for spin compensation of chromium local moments in molybdenum, in order to determine whether T_K behaves in this transition host metal as it does in a noble host metal like gold. A few trial alloy samples of this system have been completed.

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2. PLASMAS AND APPLIED ELECTROMAGNETICS

2.1 PLASMAS

2.1.1 Resonances and Wave Conversion Below the Second Electron Cyclotron Harmonic

GK 4066, National Science Foundation
AF-AFOSR-69-1622A, Joint Services Electronics Program
H. Kuehl, B. O'Brien

Several absorption lines below the electron cyclotron harmonics have been reported by Buchsbaum and Hasegawa[1,2] when the positive column of an arc discharge in an axial magnetic field was subjected to a microwave field in a cavity. Quite good agreement was obtained when the position of these lines was compared to those predicted by an approximate theory[1,2] based on an expansion in (r/l) and (r/λ) of the exact solution of the Vlasov equation. Subsequently, Pearson[3] derived more rigorous equations and compared the experimental and theoretical line positions using a more realistic density distribution than that of Buchsbaum and Hasegawa. Again, good agreement was found.

Another important aspect of these resonances is their coupling to the external field. The first treatment of the coupling was given by Stix[4] on the basis of a simplified fourth-order equation for weakly-inhomogeneous plasmas. On the basis of the Pearson equations, Kuehl[5] subsequently treated the coupling in an inhomogeneous half-space. We describe below results which have been obtained regarding the inhomogeneous half-space and the slab.

In the treatment of reflection of transmission of waves in a half space or a slab, it is possible to use two different approaches. The simplest is the cold-plasma approach in which the thermal velocities of

the plasma particles are ignored. The more correct approach is to include the thermal effects by the use of a kinetic equation. A comparison of the results of the two approaches for an inhomogeneous half-space shows that the fast-wave fields are identical if losses are small. However, in the cold-plasma approach, the energy loss from the fast waves is attributed entirely to collisional absorption very near the hybrid resonance point rather than excitation of longitudinal waves. The identity of the fast-wave fields in the two approaches follows whenever there is no longitudinal wave with power flow toward a hybrid resonancepoint. Thus, the cold-plasma results hold for a plasma slab if the longitudinal wave is sufficiently damped due to collisions.

By including thermal effects in the inhomogeneous half-space problem, it has been shown that the mode conversion between fast and slow waves is quite inefficient provided the spatial density variation near the hybrid resonance is large in a free-space wavelength.[5] This is in contrast to the results of Stix[4], who predicts that complete mode conversion takes place between a slow and fast wave. However, the results of Stix are valid only for slowly-varying densities which are usually not found in laboratory plasmas.

In the case of an inhomogeneous slab, the inefficient coupling between the fast and slow waves leads to very high-Q resonances within the plasma. We have studied the resonance line widths by using the Pearson equations.[3] We have shown that the line width is determined primarily by the density gradient at the hybrid resonance points if collisional effects are sufficiently small, and primarily by collisional effects if these effects are large.

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2.1.2 Wave-Wave Interactions in a Plasma

GK 4066, National Science Foundation

B. B. O'Brien

Wave-wave interactions in an isotropic plasma column are being investigated in the microwave frequency range. In particular, an experimental study of parametric amplification in an "up convertor" is being investigated. Initial results do not show much hope for a technically useful device, however, it is expected that quantitative measurements of preturbed electron density can be obtained.

In an initial experiment, two microwave signals (one at 900 MHz and 2 watt the other at 930 MHz and 2 mW) are incident on a positive column resonant (in the Tonks Dattner mode) at these frequencies. The amplitudes of signals at 1830 and 30 MHz have been measured. They are about 40 db down from the maximum value expected in an ideal lossless sytem as predicted by the Manley-Rowe relationships. No estimates of the losses in the experimental plasma have yet been made, thus precluding a comparison with experiment.

2.1.3 Excitation of Gas Acoustic Modes by Plasma Motion in a Magnetic Field

GK 4066, National Science Foundation

D. J. Albares

An investigation is being carried out of the excitation of gas acoustic modes by crossed electric and magnetic fields in the extended negative glow plasma[1]. The dynamics of the neutral component of a plasma and its coupling to the charged components has had little experimental or theoretical attention. Previous measurements of the electrical conductivity in this plasma in a magnetic field have been performed yielding electron-ion, electron-atom, and ion-atom momentum transfer interactions.[2] They were made at frequencies many times the fundamental acoustic frequencies in order not to excite these modes. The intention

here is to extend those measurements to lower frequencies where strong excitation of acoustic modes is anticipated.

Preliminary theoretical work upon a model of the negative glow plasma in a magnetic field has been completed and indicates that excitation of gas acoustic modes will be reflected in the electrical conductivity measurements. Acoustic oscillations, magnetic effects, and ion and electron momentum transfer interactions can be inferred in various regimes of operation accessible to the negative glow plasma. In addition to the electrical conductivity, gas pressure fluctuation and spectral line envision will be measured independently for evidence of gas acoustic motion.

Experimental work completed includes the assembly of an ultra-high vacuum system and an investigation of various cathode designs in small version of the negative glow plasma tube. Construction and procurement of all auxillary appratus and measuring instruments have been accomplished. Fabrication and assembly of the final version of the plasma tube is in progress.

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3. INFORMATION SCIENCES

3.1 CONTROL SYSTEMS

3.1.1 Stochastic Control Systems

AF-AFOSR-67-1029, Air Force Office of Scientific Research

D. D. Sworder

Several investigators have studied the possible effect of introducing into a communication system an auxiliary link from receiver to transmitter ([1] through [3]). It has been shown that if there is no noise in the feedback channel, system performance may be significantly improved with no corresponding increase in the mean power required at the transmitter. Noise in the feedback both complicates the analysis and causes deterioration in performance. Yet even here improved performance has been attained.

Of particular interest are [1] and [2]. In [1] Omura began his analysis under the premise that the receiver had a fixed linear form. With a noiseless feedback channel and uncorrelated additive noise in the forward channel, an explicit expression was obtained for the transmitter signal sequence which minimizes the mean square error between a real random variable θ and the output of the receiver after N signals have been received.

Omura solved the noisy feedback problem expediently through the application of the separation principle of stochastic control theory. The form of the transmitter signal sequence remained the same with the conditional mean of the receiver state replacing the no longer observable receiver state.

In [2] the requirement that the receiver have fixed form was removed. Instead, the transmitter and receiver were required to have certain linearity properties. In order to obviate the need for a priori

data, the receiver generated the maximum likelihood estimate of θ. Using a quadratic error measure, Butman gives explicitly the optimum transmitter signal sequence if there is no noise in the feedback channel and if the noise in the forward channel is "white".

The problem posed by Butman is no longer tractable if there is noise in the feedback channel. Bounds on performance are provided in [2] and a suboptimal coding algorithm is derived which appears relatively close to the optimum linear code.

In the past reporting period a problem similar to that examined in [1] and [2] was investigated. In contradistinction to these references only transmission of Gaussian random variables was studied. The starting point of the investigation was a derivation of the dynamical equation of the receiver. The properties of this dynamical equation were then used to deduce a structural property of the transmitter which holds for a class of communication systems without noise in the feedback channel. Some insight was gained into the effect of a priori distributions which were not Gaussian.

Using a quadratic performance measure, noisy feedback was investigated. It was shown why the separation theorem used by Omura did not apply to the problem in the form of this investigation. An asymptotically optimal transmitter sequence was derived for a system with small noise variance in the feedback channel.

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3.1.2 Fuel Optimum Space Vehicle Attitude Control

NGR 05-018-044, National Aeronautics and Space Administration

H. J. Payne, V. G. Robinson

The determination of an optimal controller for space vehicle attitude reduces to the solution of a nonlinear partial differential equation. Means of numerical solution are now available. The remaining technical problem is the development of a more efficient numerical scheme.

The most recent efforts involved the investigation of the relation of computation time to the accuracy of switching points for the optimal controller. A technique of speeding computation was developed. This produces results approximately three times faster than conventional means. In this technique calculations begin with a coarse spatial grid (resolution of switching points) which allows rapid calculation. Then refinement in the switching point is achieved by refining the solution for a finer, and smaller, grid. This is continued until sufficiently accurate solutions are determined.

3.1.3 Aggregate Variable Models of High Density Freeway Traffic

AF-AFOSR 69-1622A, Joint Services Electronics Program

H. J. Payne

The successful design of freeway traffic control systems will depend to a great extent on the development of traffic models particularly suited to the control problem. Since the status and performance of a freeway traffic system is most aptly described in terms of flow rate, density and average vehicle speed, models employing these variables--called aggregate variable models--are specially suited for this purpose.

Basically, the models consist of (1) the conservation of cars equation

$$\rho_t + q_x = f(x,t)$$

where ρ is the density, q the flow rate, and f(x,t) is the on-ramp or off-ramp flow rate; and (2) a dynamical equation. One such model discussed in [1] is given by

$$\frac{du}{dt} = -\alpha\left[\frac{q - Q(\rho) - \nu\rho_x}{\rho}\right]$$

where u is the average vehicle speed, related to the flow and density by

$$q = \rho u$$

$Q(\rho)$ is the equilibrium flow rate for density ρ, ν is an anticipation parameter and α is related to driver reaction time.

Stationary traffic patterns can be readily examined. Those existing in the region near a bottleneck have also been investigated. Breakdown of the traffic flow is predicted under certain conditions.

One general phenomenon predicted by the theory is the instability of uniform traffic flow at traffic density above some critical value.

Implementation of this model requires that it be made compatible with computational techniques available. Specifically, this requires that a spatially discrete version of the model be developed. Current efforts are centered on this problem.

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3.1.4 An Optimal Stochastic Control Problem with Observation Noise

NGL-05-018-044, National Aeronautics and Space Administration

N. E. Nahi, C. A. Cooper

Sometimes a controller is required to regulate a dynamic system under conditions where information concerning the state of the system may be difficult to obtain. This suggests the attachment of a cost to the act of observing the state. The controller should then be permitted to decide what observations to make as well as deciding what controls to use.

It will be supposed that the dynamic plant can be described by a linear difference equation, possibly driven by a stochastic input. Those observations which are made will be a linear combination of the state and possibly observation noise. When an observation is made at any sample time, an observation cost which may be a function of the sample time is incurred.

Aoki and Li[1] consider a similar problem with time invariant observation cost. Their approach is to first determine the optimal number of observations, and then determine how these observations are to be spaced in time. Our approach is to solve a Dynamic Programming functional equation for the optimal observation strategy. Following this approach, the optimal number of observations and the optimal time spacing pattern are determined simultaneously. Also, it is practically unavoidable that the optimal control strategy should be determined at the same time. Though the optimal control strategy is well known, see Chen[2] for instance, it is repeated here so as to clarify the relation between gains in the optimal observation strategy and certain gains in the optimal control strategy. Others[3-5] have considered related problems where observations are randomly interrupted.

An example is provided in which the optimal observation

strategy is determined for a particular system. Changes in the optimal observation strategy caused by changes in system parameters are illustrated. Of particular interest is the relation between the optimal observation strategy and the variance of additive observation noise.

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3.1.5 Optimal Detection-Directed Recursive Estimation

NGL-05-018-044, National Aeronautics and Space Administration

N. E. Nahi, J. C. Diebel

Discrete linear filtering theory, as developed in the past decade, has been primarily concerned with the problem of estimating the state of a linear system forced by random noise, given a sequence of noisy observations of the state. In practice, however, these observations may or may not contain information relevant to the estimation process. Specifically, there may only be an a priori probability p(k) that the

observation at the k^{th} sample time contains information on the state and a probability 1-p(k) that this observation contains pure noise. Nahi[1] was apparently the first to consider this problem from the standpoint of recursive state estimation, allowing each observation to contain signal and noise or noise alone independent of the situation for any other observations. His work is concerned with the derivation of a one-step predictor which minimizes a specialized risk function, defined as a double expectation of a quadratic cost. One of these expectations is an averaging over the plant and observation noises while the other is an averaging over the presence or absence of signal in the observation vector. The independent evaluation of these two expectations results in a linear filter as the optimal estimator for the risk function considered (i.e., the estimate, $\hat{x}(k+1)$, of the state vector, $x(k+1)$, is a linear function of the observations $y(0), y(1), \ldots, y(k)$).

A variation of the "uncertain observation" problem above is the case where it is known that with probability p all members of a given sequence of observations contain signal and that with probability 1-p no members of the sequence contain signal. This problem has also been considered as a recursive estimation problem[1], where the optimal filter is again linear by virtue of the specialized nature of the risk function. Middleton and Esposito[2] have obtained the optimal solution to the latter problem for a more general risk, but in a nonrecursive form useful only for fixed-interval estimation. The risk minimized in reference 2 is a single expectation of a quadratic cost, with the expectation taken jointly over all the random elements of the signal and observation processes, including the (random) presence or absence of signal in the observation. This optimal estimator is given in rather general form which allows the noise sources to be non-gaussian and/or the plant to be nonlinear. (Of course, the explicit evaluation of the optimal solution for these cases is, in general, more difficult.)

In this paper we discuss the optimal solution, for a general quadratic risk, of the signal estimation problem where for each sample

time the observation may or may not contain signal, independent of the situation for other observations. This filter is shown to be, in general, nonlinear and highly impractical to implement. The risk function is then redefined into a form suitable for the derivation of a detection-directed estimation procedure, whereby the outcome of a detection operation on the observation directs the manner in which the observation is used by the estimator. Optimization of the detection threshold at each sample time in the face of the ensuing estimation process is the principal result of the work described here. Computer simulations have shown that this detection-directed recursive estimator gives good results over a wide range of system parameters (signal-to-noise ratios, a priori probabilities of signal, etc.).

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3.1.6 Investigations on Necessary Conditions for Optimal Control Problems

AF-AFOSR-67-1029B, Air Force Office of Scientific Research

AF-AFOSR-69-1622A, Joint Services Electronics Program

L. W. Neustadt, K. Makowski, H. Buehler, L. S. Yeh

The principal objective of the research described in this report was to find general necessary conditions for optimization--and in particular, optimal control--problems. Results in some related areas were also obtained.

A paper[1] was completed in which there were described

results on the operator equation $x = Tx$ which were obtained in the previous six-month period, and which were described in the previous progress report. The results of this investigation were also presented at the Fifth International Conference on Nonlinear Oscillations held in September in Kiev, USSR[2].

The applications of the above-described results to optimal control theory--which provide a very general and quite natural way of extending the Pontryagin maximum principle to a very wide class of optimal control problems--were described (by L. W. Neustadt) at two conferences: a Conference on Optimization held in Nice, France in July, and a Conference on Mathematical Methods of Optimal Control and Minimal Surfaces held in Tbilisi, USSR in September. A written paper for the proceedings of the first-named conference is in preparation.

Rough drafts of three chapters of a book on "Optimization. A Theory of Necessary Conditions" (by L. W. Neustadt) were completed.

Research was begun by K. Makowski on finding necessary conditions for optimal control problems with infinite-dimensional equality constraints. Research on existence theorems for optimal control problems, using the results of [1], was begun by L. S. Yeh.

Investigations by H. Buehler on necessary conditions for optimal control problems for problems with functional differntial equation restrictions were essentially completed, and will now be written up in the form of a doctoral dissertation.

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3.1.7 Structural Problems in Linear System Theory

AF-AFOSR 69-1622A, Joint Services Electronics Program

L. M. Silverman

Let S be a linear dynamical system represented by the equations

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t)$$

where $x(t) \in R^n$, $u(t) \in R^r$, $y(t) \in R^m$ and the matrices A, B, C and D are of compatible order. In the past several years considerable insight into the structure of linear systems of the type S has been gained. In particular, such concepts as controllability, observability, stability and system equivalence are now well understood, as are their applications in many areas of control and estimation. However, there are many structural properties which are only recently beginning to be explored and appreciated. Our present research is directed towards a comprehensive study of these properties and their applications.

The main problem of interest at this time is that of feedback decoupling. This problem may be posed as follows: For a given output partition $y_1, y_2, \ldots, y_s$, where each y_i contains one or more of the components of y, when does there exist a feedback law of the form $u = Fx + Gv$ such that in the closed loop system y_i is unaffected by variations of v_j, $j \neq i$, where $v_1, v_2, \ldots, v_s$ is an appropriate partition of the new input vector v. It is further required that the closed loop system be at least output controllable to avoid degenerate cases. Several approaches to this problem have been taken[1-5] and various special cases have been effectively solved but the general problem is still open. Our preliminary investigations have revealed that a new approach based on a generalization of recently presented algorithm for system inversion[6], may lead to a complete constructive solution to the decoupling problem. Several new results have already been obtained including a complete solution for the case where G is required to be nonsingular.

The above mentioned algorithm also appears to be fundamental to the solution of many other system problems, including spectral factorization, colored noise filtering and input disturbance isolation. Work is presently in progress on these problems.

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3.2 COMMUNICATION AND RADAR SYSTEMS

3.2.1 On the Enumeration of Finite State Synchronous Sequential Machines

DA-AROD-31-124-G-1045, U.S. Army Research Office, Durham

I. P. Bottlik and I. S. Reed

I. Introduction

If in an arbitrary system one finite state synchronous sequential machine can be replaced by another finite state synchronous sequential machine such that the operation of the arbitrary system is not affected, then, intuitively, the two machines may be considered to be the same machine. The aim of this research is to determine the number of distinct (in the sense described above) machines.

Evidently if no bound is placed on the number of internal states, input states, and output states there is an infinite number of distinct machines. Hence, we consider the number of distinct machines having n input states, m output states, and no more than K internal states. The total number of representations (flow-table or state-diagram[1]) for these machines is given by:

$$T(K,n,m) = \sum_{k=1}^{K} (km)^{kn} . \qquad (1)$$

2. Equivalence Relationships

Now we may or may not allow the input and output lines of the machines to be suitably rewired when we replace one machine by another machine. Hence, we have formally defined the equivalence relations, equivalence and functional equivalence, corresponding respectively to the above two cases. Thus the number of inequivalent machines (functionally inequivalent machines) having n input states, m output states, and no more than K internal states is the number of distinct machines with (without

allowing) the input and output lines to be rewired.

Furthermore we may consider the number of distinct machines having k internal states, m output states, and n input states with and without allowing the rewiring. We have termed the equivalence relationships corresponding to these two cases permutational equivalence and isomorphism, respectively.

A machine M(k,n,m) having k internal states, n input states, and m output states is said to be minimal if there exists no machine $M_2(k_2,n,m)$ with fewer internal states ($k_2 < k$) such that M_2 is functionally equivalent to M.

We have proven the following relationships among the various equivalence relationships.

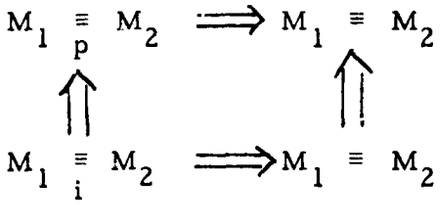

Figure 1. Relationships Between Equivalences

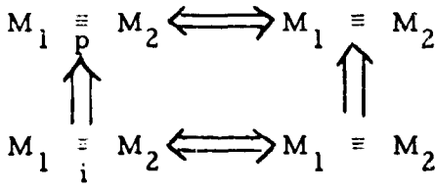

Figure 2. Relationships Between Equivalences for Minimal Machines

We have also shown that the number of inequivalent, functionally inequivalent machines having n input states, m output states, and no more than K internal states is given by:

$$E(K,n,m) = \sum_{k=1}^{K} p(k,n,m)$$ where p(k,n,m) is the number of permutationally inequivalent minimal machines having k internal states, n input states, and m output states; (2)

$$F(K,n,m) = \sum_{k=1}^{K} i(k,n,m)$$ where i(k,n,m) is the number of non-isomorphic minimal machines having k internal states, n input states, and m output states; (3)

respectively.

3. Group Machines

The class of machines considered may be restricted to a subset of the finite state synchronous sequential machines. In particular, we have considered Group Machines, which are those finite state synchronous sequential machines for which the next state function $f: S \times X \rightarrow S$ is a one to one mapping of the internal states, S, onto the internal states, S, for each input state $x \in X$. The total number of representations of group machines having n input states, m output states, and no more than K internal states is given by:

$$T'(K,n,m) = \sum_{k=1}^{K} (k!)^n m^{kn} \quad . \tag{4}$$

The relationships of Fig. 1, Fig. 2, (2) and (3) are applicable to group machines (i.e., machine is to be replaced by group machine).

4. Strongly Connected Group Machines

The class of machines considered may be further restricted. In particular, we have considered strongly connected group machines, which are those group machines for which every internal state can be reached from any internal state by some sequence of input states.

The relationships of Fig. 1, Fig. 2, (2) and (3) are applicable to strongly connect group machines.

5. Enumeration Formulas - Permutational Equivalence of Machines

We have rigorously proven a result due to Harrison[2] and Harary[3]. Namely, the number of permutationally equivalent machines having k internal states, n input states, and m output states is given by:

$$P(k,n,m) = \frac{1}{k!n!m!} \sum_{a \in S_k} \sum_{b \in S_n} \sum_{c \in S_m} h(a,b,c) \qquad (5)$$

where 1) $h(a,b,c) = \prod_{p=1}^{kn} \left[\sum_{q|p} q \cdot j(q,a) \cdot \sum_{q|p} q \cdot j(q,c) \right]^{f_1(p,a,b)}$;

2) $f_1(p,a,b) = (1/p) \sum_{\substack{s,t \\ sp=\mathrm{lcm}(s,t)}} j(s,a) \cdot j(t,b) \cdot s \cdot t$;

3) $V_i \geq 1$ $j(i,a)$, $j(i,b)$, $j(i,c)$ is the number of cycles of length i in the disjoint cycle decomposition of a, b, c respectively;

4) S_k, S_n, S_m is the symmetric group on k, n, m elements, respectively;

5) $\mathrm{lcm}(s,t)$ is the least common multiple of s and t.

The number of non-isomorphic machines follows directly from the above formula by letting S_n, S_m be the group consisting only of the identity element acting on n, m elements respectively.

6. Permutational Equivalence of Group Machines

We have proven that the number of permutationally inequivalent group machines having k internal states, n input states, and m output states is given by:

$$P'(k,n,m) = \frac{1}{k!n!m!} \sum_{a \in S_k} \sum_{b \in S_n} \sum_{c \in S_m} h_1(a,b)\, h_2(a,b,c) \qquad (6)$$

where 1) $h_1(a,b) = \prod_{p=1}^{n} \left[\sum_{q \mid p} q \cdot f(q,a) \right]^{j(p,b)}$;

2) $h_2(a,b,c) = \prod_{p=1}^{kn} \left[\sum_{q \mid p} q \cdot j(q,c) \right]^{(1/p) \sum_{s,t \ni p = lcm(s,t)} j(s,a) \cdot j(t,b) \cdot s \cdot t}$

3) $f(q,a) = (1/q) \cdot \sum_{s \mid q} \mu(q/s) \left[\prod_{t=1}^{k} t^{g(t,s,a)} \cdot g(t,s,a)! \right]$;

4) $g(t,s,a) = 1/t) \cdot \sum_{u \ni u = gcd(s,t)} u \cdot j(s,a)$;

5) gcd(s, t) is the greatest common divisor of s and t;

6) j, lcm are as defined in section 5;

7) μ is the Mobius function.

The number of non-isomorphic group machines follows directly from the above formula by letting S_n, S_m be the group consisting only of the identity acting of n, m elements, respectively.

7. Functional Equivalence of Strongly Connected Group Machines

We have proven that the number of functionally inequivalent strongly connected group machines having 1 input states, 2 output states, and no more than K internal states is given by:

$$F''(K,1,2) = \sum_{k=1}^{K} n(k)/k \ , \qquad (7)$$

where: $n(k) = 2$ if $k = 1$

$$= 2^k - 2 - \sum_{a=1}^{k-1} \sum_{\substack{p>1 \\ p \mid \gcd(a,k-a)}} m(a/p, (k-a)/p) \text{ if } k > 1$$

$$= 2^k - 2 \text{ if } k \text{ is prime .}$$

Also $m(a/p, (k-a)/p)$ can be calculated by the recursion formula

$$V_{s,t} > 0 \quad m(s,t) = \binom{s+t}{s} - \sum_{\substack{p>1 \\ p \mid \gcd(s,t)}} m(s/p, t/p) .$$

8. Computer Programs

Computer programs have been written to check the formulas (5), (6), and (7) for small values of k, n, m. Furthermore, programs have been written which calculate the number of inequivalent machines, E(k, n, m), the number of inequivalent group machines, E'(k, n, m), and the number of functionally inequivalent group machines, F'(k, n, m), for small values of k, n, m. All of these programs are essentially an exhaustive search to determine the number of distinct machines. Results of these programs are indicated in Table 1 by c.

9. Numeric Results

For certain small values of k, the number of internal states n, the number of input states, m, the number of output states the number of distinct machines, group machines, strongly connected group machines are given in Table 1. Values calculated by the computer programs (essentially an exhaustive search) are denoted by c. Values calculated by the formulas are indicated by f. Values T, T' are also given to show the drastic difference between the number of representations and the number of distinct machines.

Table 1 - Legend

k - number of internal states, or bound on the number of internal states.

n - number of input states.

m - number of ouput states.

$T^* = T(k) - T(k-1)$ - total number of representations of machines with k, n, m states.

E - number of inequivalent machines having no more than k internal states.

F - number of functionally inequivalent machines having no more than k internal states.

P = number of permutationally inequivalent machines.

' - denotes group machines.

'' - denotes strongly connected group machines.

f - calculated by formula (5), (6), or (7).

c - as determined by computer program doing an exhaustive search.

Table 1 - Numeric Results

kmn	T*		E		P	T'*	E'	F'	P'		F''
112	2	c	1	fc	1	2	c 1 c	2	fc 1	fc	2
212	16	c	4	fc	6	8	c 3 c	4	fc 4	fc	3
312	216	c	10	fc	22	48	c 5 c	8	fc 7	fc	5
412	4096	c	32	fc	114	384	c 8 c	16	fc 20	fc	8
512	100000	c	102	fc	508	3840	c 16 c	32	fc 37	fc	14
612	2995984			fc	2800	46080	c 34 c	64	fc 90	fc	23
712				f	14435				f 175	fc	41
812									f 390	fc	71
912									f 773		
122	4	c	2	fc	2	4			fc 2		
222	256	c	32	fc	44	64			fc 16		
322	46656	c	1556	fc	2038	2304			fc 124		
422	16777216			f	176936	147456			fc 1770		
522				f	3048092				f 32190		
111			1	fc	1	1		1	fc 1		
211			1	fc	3	1		1	fc 4		
311			1	fc	7	1		1	fc 7		
411			1	fc	19	1		1	fc 20		
511			1	fc	47	1		1	fc 37		
121			1	fc	1	1		1			
221			1	fc	7	1		1			
321			1	fc	74	1		1			
421			1	fc	1474	1		1			

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3.2.2 k-th Order Near Orthogonal Codes

DA-AROD-31-124-G-1045, U.S. Army Research Office, Durham

I. S. Reed

Recently, certain near-orthogonal codes have been used and proposed for multiple frequency shift keying (FSK) communications systems. The codes most generally considered for this application are the first order Reed-Solomon (RS) codes. These codes have the property that no two members of the code overlap in more than one symbol or frequency-time (FT) slot, and as a consequence are very nearly orthogonal.

The purpose of this research is first to show that the above class of codes can be extended to a code with the property that no two members of the code overlap in more than k frequency-time slots. These codes have been designated k-th order near orthogonal codes. Finally, it has been shown that certain subsets of k-th order near orthogonal codes can be generated in such a manner that no two words of a subset under different time delays or translations overlap in more than k symbols. The latter property means that these codes can be detected asynchronously with a bank of matched filters (either coherently or noncoherently). It is in this sense that these subsets constitute a self synchronizable or comma free codes. These codes have been termed synchronizable k-th order near orthogonal codes.

3.2.3 Information Rates of Autoregressive Processes

DA-ARO-D-31-124-G-1045, U.S. Army Research Office, Durham

R. A. Scholtz and R. M. Gray

The rate distortion function, R(D), of a source can be interpreted as being the average amount of information that must be transmitted about a source for the receiver to be able to approximate the source within an average distortion D. It has been demonstrated[1] that for the class of time discrete autoregressive sources the rate distortion function for any difference distortion measure is lower bounded by the rate distortion function of the independent letter source that generates the autoregressive source. Autoregressive sources are constructed by passing such an independent letter source through a time discrete linear filter whose z-transform has only poles. This behavior holds even if the autoregressive source is nonstationary. The lower bound is shown to hold with equality for a nonzero range of small average distortion for two important special cases: the class of possibly nonstationary Gaussian autoregressive processes with a mean square error fidelity criterion and the binary symmetric first order Markov source with an average error per bit fidelity criterion.

Similar results have been obtained for the case of an independent letter Gaussian source passed through a more general linear filter for the time continuous Gaussian autoregressive process. Finally, some original results on the asymptotic behavior of the eigenvalues of Toeplitz and approximately Toeplitz matrices have been obtained.

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3.2.4 Codes for Almost Sure Synchronization

DA-ARO-D 31-124-G-1045, U.S. Army Research Office, Durham

R. A. Scholtz and R. M. Storwich

A fundamental requirement for the operation of a digital communication system is the ability to establish and maintain synchronization (sync) between transmitter and receiver. If the receiver begins its operation with no knowledge of true word sync, it must be found before any information can be transmitted. When the message sequences to be transmitted are very long (or infinitely long) and received noiselessly, the system may be designed to use the shortest possible codewords in order to maximize the transmission rate. Under these conditions the sync procedure must operate in a statistical manner, since the maximal dictionary size permitted for the existence of a bounded sync delay procedure for codewords of this length is generally exceeded. The relevant considerations in developing a statistical sync procedure have been studied, and a particularly advantageous approach selected for further development.

Basically, this synchronizer inspects the code symbol stream for the first occurrence of an event (e.g., a fixed finite length code symbol sequence) which appears in only one position relative to true word sync. This position-characteristic sync event enables the immediate establishment of word sync. The receiver can then make unambiguous sync decisions for almost every code symbol sequence it may receive, and can be realized easily by using simple shift register constructions. Result on the range of the average sync delay for optimally encoded sources have been determined.

When the sync event is the appearance of a fixed finite sequence, the effects of changing its structure are investigated. In particular, when the sync sequence has the same length as the codewords, the structural conditions needed to allow the dictionary to contain the most useful code-

words have been found. The maximal number of codewords in this choice of dictionary has been determined and shown to depend upon the sync sequence's position. This makes it possible to choose the best sync sequence position for a given message source. A class of sequences with this desired structure has been found.

The manner with which the probability of not having established sync approaches zero is of interest. It provides a criterion for comparison of statistical sync processes which cannot necessarily make unambiguous sync decisions. For the sync procedure developed, the exact behavior of this probability has been shown to have the expected exponential form. Upper and lower bounds to this probability have been derived and also shown to have exponential forms. Further, these bounds may be partially characterized by the average sync delay.

A method for analyzing the ultimate sync capabilities of a given dictionary has been developed and used in an example to indicate the efficiency of the single position sync event method. This method of analysis utilizes another relatively simple manner of statistical sync which also applies to nonuniform length dictionaries.

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3.2.5 Signal Design for the Noncoherent Gaussian Channel

DA-ARO-D 31-124-G-1045, U.S. Army Research Office, Durham

M. S. Stone and C. L. Weber

A fundamental problem in Communication Theory is the design of M-ary communication systems. Our interest here is with the signal design portion of the problem for the noncoherent additive white Gaussian noise channel. The signalling waveforms under consideration are assumed to consist of M equiprobable, equipowered narrowband waveforms of signal time duration.

The mathematical model for the noncoherent communication system and a general representation of the resulting probability of error as a function of signal-to-noise ratio and an arbitrary set of narrowband signalling waveforms has been previously described.[1]

In our work, a simplified approximation to the error probability has been derived for high signal-to-noise ratios. With this expression, it is shown that the noncoherent orthogonal signal structure globally minimizes the probability of error at large signal-to-noise ratios when the dimensionality of the signal set is unrestricted.

The dimensionality constrained signal design problem was then considered. The problem of finding optimal signal sets of given dimension was formulated as a variational one. This leads to a necessary condition that must be satisfied so as to locally extremize the error probability. It was then shown that for dimensionality restricted by

$$D \leq 2M-K$$

where

$$K \leq 2[M/3] ,$$

where [ ] denotes the "integer part of", and $M \geq 6$, signal inner product matrices consisting of K regular simplicies placed mutually orthogonal to

one another are local extremals of the probability of error. Of the several solutions for each K, the most preferred one was selected for large signal-to-noise ratios.

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3.2.6 Stochastic Optimization of Coherent Communication Systems in Additive White Gaussian Channels

DA-ARO-D 31-124-G-1045, U.S. Army Research Office, Durham

S. Moskowitz and C. L. Weber

A basic signal design problem in communication theory is that of determining the signal set $\{\bar{S}_j\}$ which minimizes the probability of error, and further, of determining the dependence of the optimal signal set on the signal-to-noise ratio. This problem, also known as the signal selection problem, can be reduced to that of finding a set of M vectors in D-dimensional space which maximizes the detection probability functional. For equal energy constraints on the signals to be transmitted, the problem is further reduced to M unit vectors on a D-dimensional sphere.[1]

Notable analytical contributions have been made toward the solution of this problem.[1] However, results exist mainly for equi-likedly, equal energy signals and for $2 < D < M/2$, the problem is still open. Furthermore, where the a priori probabilities of transmission are known, essentially no results exist at intermediate signal-to-noise ratios.

A different approach to this long unsolved problem has been taken in this research. Since we are concerned with maximizing a functional subject to a constrained signal set, known gradient techniques may be applied to obtain at least local maxima. This, of course, assumes sufficient smoothness properties of the functional with respect to the signal coordinates, properties which heretofore the detection probability functional has been shown to possess. In particular, the probability of detection is analytic with respect to the signal set's angular space coordinates. Hence, maxima of the probability of detection can be obtained using gradient methods and this is in fact the approach taken here. The gradient vector of the probability of detection is in general not expressible in closed form. It can be approximated, however, using Monte Carlo methods since the probability of detection can be shown to be an expectation of an exponential function of a D-dimensional Gaussian random variable.

The application of gradient techniques to obtain approximate solutions to the problem has been formulated and run on an IBM 360 Computer. Convergence to local optimal points has been demonstrated. Results obtained have corroborated known solutions or have provided new solutions (in an approximate sense) for D = 2, 3, 4 regardless of energy constraints or a priori probabilities. In some cases, analytical verification of first or second order conditions for optimality has also been established. Furthermore, once the vector solutions have been obtained, a one-to-one correspondence between this and corresponding time solutions can be established.

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3.2.7 Multipath Considerations in Sonar Detection

DA-ARO-D 31-124-G-1045, U.S. Army Research Office, Durham

W. J. Busch and C. L. Weber

In active sonar detection the effects of reverberation, background noise and multipath returns are of varying significance depending on the ocean conditions and depth. This research is concerned primarily with active sonar detection in shallow water regions where multipath returns are a predominant effect. Instead of trying to cancel out the effects of multipath, this paper considers the multipath returns together with the direct return as forming a composite signal. The direct portion of the composite signal is taken to be narrowband with random amplitude and phase. Due to the severe distortion encountered on bottom-bounced the multipath returns are modeled as a series of pulses which are segments of independent gaussian random processes. For analytic simplicity it is assumed that the arrival times of the direct signal and the multipath pulses are known.

Employing this composite signal model, the optimal detector in the Neyman-Pearson sense is developed. It has been found that this detector involves weighting functions which are solutions of certain integral equations. To avoid the difficulties associated with this, an approximate detector was developed which does not require the solution of any integral equations. The resulting detector is a combination of a narrowband signal detector and a series of stochastic signal detectors, and hence is called the composite detector.

The performance of the composite detector is evaluated by obtaining the probability of detection for a given probability of false alarm. The general results are applied to a particular example in order to obtain some typical numerical results. These results indicate that under certain conditions, the presence of multipath can greatly enhance the probability of detection. Hence, it has been shown that multipath considerations can

be very significant in active sonar detection.

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3.2.8 Specification and Performance Evaluation of Optimal State Variable Filters for Communication Problems

DA-ARO-D 31-124-G-1045, U.S. Army Research Office, Durham

D. C. Beste and C. L. Weber

One of the fundamental problems of analog communication theory is that of determining the structure of the best implementable receiver for a stochastic signal process which amplitude, frequency, or phase modulates a sinusoidal carrier signal.

The approach that has been taken to solve this optimal realizable nonlinear filtering problem has been to first determine, using a nonlinear state variable approach, the exact mathematical formulation of the optimum realizable least mean square error signal estimator, and then to consider several types of approximations which lead to practical physically realizable demodulators. It has been shown that when the appropriate communication engineering considerations are taken into account all of the various approximation schemes reduce to similar forms. The minor differences in the approximately optimum demodulator formulations suggest which parameters should be investigated to determine if the specified demodulator is locally optimum.

A study is currently being undertaken to evaluate the performance of the specified optimal demodulators and to determine the effect of missmatched parameters.

3.2.9 Pioneer VI Solar Faraday Rotation Experiment

Partially sponsored by Grant GU 1559, National Science Foundation

J. E. Ohlson, W. V. T. Rusch, C. T. Stelzried

A. Introduction

In November 1968, the Pioneer VI Spacecraft underwent solar occultation as it passed approximately one astronomical unit behind the sun. Before and after occultation by the visible disk, the spacecraft signals passed through the solar corona on their way to earth and experienced Farday Rotation. This effect is a spatial rotation of the plane of polarization of a linearly polarized wave when it passes through a plasma in the presence of a longitudinal magnetic field. A sensitive receiving system was developed to measure this effect, and a large amount of data was obtained during the occultation. Three startling transient phenomena were observed, and measurements of the steady-state coronal contribution were made. This experiment was performed jointly with personnel of the Communications Elements Research Section of the Jet Propulsion Laboratory, G. S. Levy, B. Seidel and T. Sato.

B. Experiment Description

During the occultation, the spacecraft was tracked with the 210 feet in diameter NASA/JPL parabolic antenna at Goldstone, California. The r.f. hardware and receivers were extensively modified to effectively provide a cross-linearly-polarized feed system which can be automatically rotated to any position. This is the heart of the system. One feed produces an error signal which is continuously driven to zero by servopositioning the feed system. The second feed is thus automatically aligned with the signal vector and provides a reference for the detection of the error signal. A pair of mechanically rotatable waveguide-section quarterwave plates is used to synthesize the effectively rotating feed system. The position of one plate is accurately fixed and the position of the other tracks the

received signal. Its position was digitally recorded and processed through a celestial coordinate conversion program to obtain the Faraday Rotation undergone by the signal.

Several factors made this a difficult experiment:

1) The signal was very weak from traversing a distance of two astronomical units.

2) Intense radio noise of the sun entering the antenna side-lobes reduced the signal-to-noise ratio and prevented following the space-craft to and from the photospheric limbs.

3) Coronal turbulence produced severe spectral broadening of the signal which made tracking difficult.

4) The earth's ionosphere contributes a rotation of 1-7^{o} to the signal. This ionospheric rotation was measured separately with a geostationary satellite and is being removed from the data.

C. Experimental Results

For several months prior to November 1968, data were taken with a manual version of the experimental system. This gave a data baseline and data on the ionosphere. Starting approximately November 1, the system was in its final form. On November 4, the first indication of solar effects was obtained. Over a period of about two hours a rotation of some 40^{o} was observed. This correlated exactly with enhanced spectral broadening of the signal measured by a second experiment. On November 8 and 12 similar events occurred, again correlated with enhanced spectral broadening. These three events appear to be correlated with decametric solar radio bursts and intense decimetric regions on the sun. A possible explanation is that a dense plasma cloud was expelled from the sun and passed between the spacecraft and the earth. As the spacecraft neared the sun (in angle) an increasing steady-state rotation was measured until solar radio noise prevented tracking of the spacecraft. After several days when the spacecraft was behind the sun, it emerged and the rotation angle was again measured. The interesting fact was that the rotation on exit

was comparable in magnitude to the entry measurements but was of opposite sign. Solar magnetic field data was obtained from corouagraphs and a fit for electron density has been obtained that does not differ considerably from the Allen-Baumbach theory. The fit obtained of free electrons per cubic meter was

$$N = 10^{14}\left(\frac{6000}{R^{10}} + \frac{.002}{R^{2}}\right), \quad M^{3}(4 < R < 12)$$

where R is in omits of solar radii.

D. Future Plans

(1) Documentation of system and results;

(2) Preparation for occultation of Pioneer IX in November 1970.

Reference

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3.2.10 Hybrid Processing of Complex Radar Signals

GK-3303, National Science Foundation

J. E. Ohlson

Work is continuing on the problems of large time-bandwidth radar signals. Great difficulty exists in the use of digital processing for signals with a large number of degrees of freedom. Effort has been expended as follows:

(1) A special class of radar signal has been developed that is a generalization of the classical chip. It does not exhibit the severe ambiguity of range-doppler that is typically found in pulse compression systems.

(2) The problem of impulsive noise is being treated in the bandpass limiter for application to radar signal limiting and coherent communication.

(3) Two special systems utilizing detection information have been analyzed that allow use of a fully phase-modulated carrier for coherent phase tracking. Performance is comparable to that of the squaring (or Costas) phase-locked loop.

3.2.11 Nonlinear Analysis and Synthesis of Generalized Tracking Systems

GU 1559, National Science Foundation
AF-AFOSR 69-1622, Joint Services Electronics Program

W. C. Lindsey, A. Chang, J. R. LaFrieda

The purpose of this research is to study fundamental problems relative to improving the performance capability and efficiency of telecommunication systems. In particular, the investigation is concerned with obtaining "time-solutions" to the Fokker-Planck equation which specifies the performance of a generalized synchronization system.[1] Such solutions have a variety of applications in practice, e.g., computation of mean time to signal acquisition, correlation functions of various

scientific measurements, etc.

Recently, results for the N^{th}-order nonlinear tracking loop have been obtained via a method similar to the Barret-Lampard expansion for first-order Markov processes.

Approximate numerical solutions of a periodic two-point boundary value problem, corresponding to the time-dependent Fokker-Planck equation, have been constructed for the transition probability density function of the nonstationary, Markov phase-error process. From these results, the steady-state autocorrelation and power spectral density functions of the phase-error process have been obtained. In addition, for the case of Nth-order loops, approximate solutions of the time-independent Fokker-Planck equation have been obtained for the phase-error process. The details of this work will be published in a forthcoming paper.

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3.2.12 Image Processing by Digital Computer

JPL 952312, Jet Propulsion Laboratory

NGL-05-018-044, Supplement #3, National Aeronautics and Space Administration

H. C. Andrews and W. K. Pratt

The Image Processing Laboratory is extensively involved in the application of digital computational techniques to image processing problems. Presently, research is underway on: image coding techniques for bandwidth compression and channel error immunity for monochome and color images; image enhancement methods for edge and contrast improvement; and pattern recognition pre-processing operations.

The basis of the image processing research is the utilization of mathematical transformations on images to achieve a desired result. These transformations may be conveniently described in terms orthogonal matrix operations on image vectors. On a digital computer, multiplying an orthogonal matrix by a data vector is equivalent to decomposing the data into a set of coefficients of the orthogonal waveforms making up the matrix. If the entires of the matrix are complex trigonometric waveforms, then the vector-matrix product is equivalent to a Fourier transform. If the orthogonal entires of the matrix are other waveforms, then the decomposition results in a generalized spectral analysis. Implementation of such decompositions in a digital computer normally require N^2 operations for a vector-matrix product. However, if there is some built-in redundancy in the definition of the matrix, then often this redundancy can be used to implement the vector-matrix product in less than N^2 operations. A class of orthogonal transformations are being investigated which are implementable in $pN \log_p N$ operations where $N = p^n$. This class of transformations has led to the fast Fourier transform, the fast Hadamard transform, the fast Walsh and Generalized Walsh transform and many other types of orthogonal transformations.[9,10] Some of these transfor-

mations have the property of compacting a large percentage of the total energy in a picture into a very few number of coefficients. This is a result of the fact that pictures of interest tend to have some degree of two dimensional correlation. If an image is grid sampled at N^2 different points, it can be expressed as a sampled function $f(x, y)$. Then the pertinent discrete two dimensional transformations described above become:

Fourier:

$$F(u,v) = \frac{1}{N} \sum_{x=0}^{N-1} \sum_{y=0}^{N-1} f(x,y) \exp\left\{ -\frac{j2\pi}{N} (ux + vy) \right\}$$

Hadamard/Walsh:

$$F(u,v) = \frac{1}{N} \sum_{x=0}^{N-1} \sum_{y=0}^{N-1} f(x,y) (-1)^{\sum_{i=0}^{n-1} u_i x_i + v_i y_i}$$

where $N = 2^n$, and u_i, x_i, v_i, y_i refer to the binary variables in the binary representation of the parameters u, x, v, y respectively. Considerable success has been achieved in using these transformations for bandwidth reduction and noise immunity coding[1-8].

Generalized Walsh Transform:

$$F(u,v) = \frac{1}{N} \sum_{x=0}^{N-1} \sum_{y=0}^{N-1} f(x,y) \exp\left\{ \frac{2\pi\sqrt{-1}}{p} \left[\sum_{r=0}^{n-1} \sum_{j=0}^{p-1} \sum_{m=0}^{p-1} jm\delta(x_r - j) \right.\right.$$

$$\left.\left. \delta(u_r - m) + \sum_{k=0}^{p-1} \sum_{q=0}^{p-1} kq\delta(y_r - k)\, \delta(v_r - q) \right] \right\}$$

where $N = p^n$ and u_r, x_r, v_r, y_r refer to the lexicographic variables in the dictionary representation of the parameters u, x, v, y respectively.

The image transforms described above have been successfully applied to monochrome images to obtain a bandwidth compression and a

certain tolerance to channel errors. A theoretical and experimental study has been undertaken to apply the transform coding method to color images. In the color image transform coding technique being investigated a linear coordinate conversion is first made on the red, green, and blue primary signals of the image sensor to obtain a luminance and two chrominance signals. The luminance signal is then processed and coded using the best available monochrome processing methods. Two dimensional image transforms are taken of the chrominance signals. Only those transform samples of a critical magnitude are coded and transmitted. Preliminary indications are that a 15: 1 bandwidth compression can be achieved by this type of coding.

In attempting to answer the question as to what processing should be done on transform samples, it is worthwhile to consider the options available. Several methods of transform sample processing are listed below:

linear filtering
- scalar
- vector

nonlinear filtering
- scalar
- vector

dynamic weighting

Linear scalar filtering simply consists of amplitude scaling, and phase scaling if appropriate, of each transform sample independently. In linear vector filtering the sample scaling is not performed independently between samples.

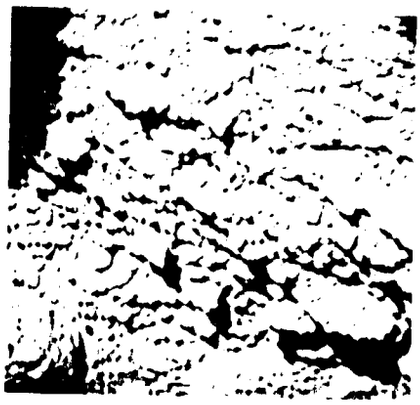
Nonlinear filtering, as defined here, consists of performing a nonlinear operation on each transform sample. For example, in nonlinear scalar filtering each transform sample might be brought to a power $1 + \Delta$ where Δ is a small number. Such an operation has the effect of emphasizing the difference between low amplitude and high amplitude samples. Another

method of nonlinear filtering consists of taking the logarithm of each transform sample. Qualitatively, this operation tends to reduce the dynamic range of samples in the transform domain and increase the dynamic range in the sample domain upon reconstruction. Bogert, Healy, and Tukey have introduced a similar transformation for speech processing as a means of detecting echoes[11]. In their transformation (called the cepstrum) the power spectrum is taken of the logarithm of the power spectrum of a signal. This concept has been generalized by Oppenheim, Schafer, and Stockham who defined the complex cepstrum as the Fourier transform of the logarithm of the Fourier transform[12]. The cepstrum can be further generalized to other transforms. For an arbitrary real transform the generalized cepstrum is defined as

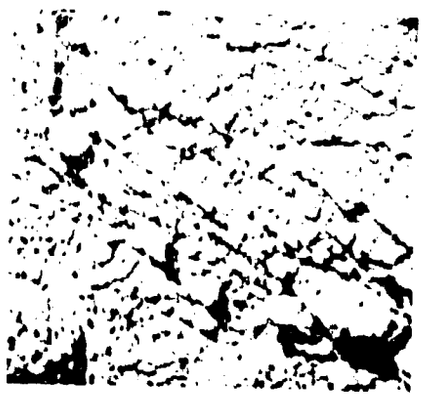
$$\hat{f}(x,y) = \sum_{u=o}^{N-1} \sum_{v=o}^{N-1} (\text{Sign } (F(u,v)) \ln \{ 1 + |F(u,v)| \} b(x,y,u,v)$$

For a complex transform such as the Fourier transform the logarithm is taken on the magnitude of the transform sample. Figure 1 illustrates an experimental result of cepstrum processing with the Hadamard transform on a moonscape. Notice that detail in the shadow of the original has been made visible and that this same detail is not seen in the example of Hadamard linear filtering.

Dynamic weighting is radical departure from the classic idea of filtering. For all of the transforms described in the previous section the fast computational algorithms provide a decomposition of a data vector in stages. For example, in the Fourier or Hadamard transform of a vector of $N = 2^n$ points where n is an integer, n vectors of data are produced in the computation. The nth vector is the complete transform. Since the transform data is available at the intermediate stages it can be modified dynamically during the computation. It is not clear that it is beneficial to perform dynamic weighting simply because there are convenient entry points to the data. However, there are heuristic reasons that



a. Linear - Conical Ramp Filter



b. Nonlinear - Hadamard Cepstrum Filter

Figure 1. Hadamard Filtering

lead to the belief that dynamic weighting may be worthwhile. In the Hadamard transform, for example, the additions and subtractions at each stage in the computation essentially provide a de-correlation of the input data vector. If the data vector represents a line of a low contrast image it may be helpful to emphasize the differences with respect to the summations to improve the overall contrast. The experimental results with Hadamard cepstrum processing tend to support this conjecture.

The use of orthogonal transforms in two dimensional digital image processing opens up an entirely new approach to the problems of image enhancement. The preliminary experimental results presented herein serve to indicate the potentiality of transform processing for image enhancement. It is also clear from the discussion that there is need for a theoretical background to adequately explain the results obtained, and possibly point towards new processing techniques.

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3.2.13 Nonparametric and Adaptive Techniques in Communication

AF-AFOSR 69-1622A, Joint Services Electronics Program

L.D. Davisson

Introduction

The purpose of this research is to investigate adaptive and nonparametric techniques as they apply to the communication, filtering, prediction, and detection of analog and digital signals. Optimal solutions or bounds on performance are sought and compared with practical, possibly suboptimal methods. Theoretical performance measures and analysis techniques are developed.

Probability of Convergence for Stochastic Approximation

An important method of system optimization, when required system parameters such as probability distributions, transfer functions, etc., are unknown, is the recursive estimation method for the desired

parameters called stochastic approximation. After each of a sequence of observations, parameter estimates are updated by making an incremental change given by a function of the current observation and current estimates only. The increment contains a gain factor which goes to zero with time in such a way that convergence to the desired value occurs under appropriate conditions.

In such stochastic approximation applications, sufficient conditions for mean square and probability one convergence are known (see for example [1]). In many cases the most difficulty of the conditions to satisfy is that of the estimate having an expected step change which increases the error norm at every point of the estimate space. One way to avoid the difficulty as given by Sakrison[1] is to restrict the estimate to values in a range where the condition is known to be satisfied. However, this may not be possible due to uncertain knowledge of the regression function and/or location of the value to which one wishes to converge. In recent research a lower bound was found on the probability of convergence when the estimate is unrestricted after starting somewhere in the region of convergence through the use of "training sequences", minimax values or other appropriate methods. The bound results from a consideration of the probability that the estimate leaves a given region of convergence at any time when left free to do so. Clearly if this event does not occur, the estimate must converge because the sequence of estimates is then the same as if boundary restrictions had been employed and hence the probability of convergence is greater than or equal to one minus this event probability. The lower probability bound can be maximized over all regions of convergence.

The results found represent a generalization of earlier work[2,3] which was tied to the specific application of estimating signal probabilities by relative decision frequencies, the probability estimates then being used in the decision structure as if they were the actual values to minimize error probability. The initial estimates were taken as the minimax values. In [2,3] it was found that the probability of nonconvergence was infinitesimal

at moderate signal-to-noise ratios (typically 10^{-4000} at a signal-to-noise power ratio of 4) although at low values convergence never occurs.

Other important applications of the work can be found in other decision directed structures (see [2] for references) in particular in adaptive channel equalization* (reference 3 of [2]). In the latter case a training sequence is used to get the initial estimates. In the reference it is found that the region of convergence is seldom left at moderate signal-to-noise ratios but no probabilities are found.

In other applications the sufficient conditions for convergence may be satisfied but one might like to know the probability of large excursions from the final value. The techniques developed can also be applied here.

Data Compression Research

Various techniques have been developed to encode source data in a manner which is hoped to be reasonably efficient and simple in implementation. A frequent fidelity criterion imposed on the techniques is that the error in reconstructing each sample value be no greater than some a priori set threshold ε. This research is concerned with the transmission rate required for some of these techniques compared with the lower bound, with respect to this fidelity criterion, known variously as the rate distortion function (of ε), information rate, or ε-entropy (with ℓ_∞ norm) of the source. Unfortunately, the bound is difficult to evaluate for other than fidelity criteria of the mean square variety. In these studies upper and lower bounds on the ε-entropy are considered. Although the results are given in terms of a stationary Gaussian source for want of a better model, other distributions could be handled as well. The upper bound is attained by a given (relatively complex) scheme. It is shown by example that this bound can be closely approximated by an optimum linear prediction scheme

*In practice the incremental gain is normally left constant in this application to allow the stimates to follow nonstationarities but the difficulties with a finite stability region still exist.

and that the performance for a given spectral density can be calculated with negligible error by assuming a normal prediction error with a variance calculated using quantized second moments only. The optimum linear predictor depends strongly on ε as well as the spectral density suggesting the use of a simple adaptive scheme. Performance comparisons are made with some simple polynomial prediction compression schemes.

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3.2.14 Automata and Communications

AF-AFOSR 68-1555A, Air Force Office of Scientific Research

S. W. Golomb and I. S. Reed

I. Progress

Papers 1) and 2), which had been submitted to the IEEE Transactions on Information Theory in June 1969, have now been accepted for publication. Meanwhile, additional work on synchronization coding is being carried out, including a) studies of optimum synchronization techniques in the presence of noise, and b) the search for optimum phase-modulated synchronization patterns.

A major paper by Dr. W. C. Lindsey, based on his two USCEE

Reports 317 and 342, listed below as Reference 4a and 4b, was written and submitted to the Proceedings of the IEEE. This paper, entitled "Nonlinear Analysis of Generalized Tracking Systems", was accepted for publication to appear in the October 1969 issued of the Proccedings (Reference 5).

The papers listed as References 9 and 11, both involving the geometric aspects of coding theory are scheduled to appear in their respective journals at the beginning of 1970. Further research along the lines of References 8, 9, 10, and 11 has been and is being performed and will be the subject of future journal articles.

II. Applicability of This Research

Our studies of efficient coding for self-sycnrhonizing communication (see References 1, 2 and 3) have led to families of codes, together with convenient encoding and decoding techniques, which are particularly well suited to channels subjected to frequent and/or unpreditable fade-out and fade-in characteristics.

An attractive possibility in military radio communications is to use a signalling alphabet based on phase modulation of an RF carrier. If n equally spaced phases are used, the appropriate error model is either the Lee Metric, as considered in 8) and 9), or one of the more general error metrics described in 10). The development of optimum coding systems for channels of this type has been the subject of a continuing research effort under this project and is reported on extensively in 8) and 9).

The research efforts reported in 5) constitute a major contribution to the theory of tracking systems, which have innumerable military applications. Lindsey's work, 5), was not only important enough to merit publication in the Proceedings of the IEEE, but actually furnishes the cover picture for the October 1969 issue in which it appears.

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3.2.15 Digital Techniques for Multi-Signal Environments

DA-AROD 31-124 G930, Supp. #1

DA-AROD 31-124-G1044, U. S. Army Research Office, Durham

S. W. Golomb and L. R. Welch

I. Brief Statement of the Problem

Maximal-length linear shift register sequences (also called "m-sequences" or "PN sequences") have found a variety of important applications to communications in an environment which is noisy, hostile, or otherwise unfavorable to reliable communications. In several of these applications, it would be highly desirable to be able to use several such signals in the same environment, as in the case of one master station communicating with several outposts at once. In order to accomplish this, it is necessary to determine the mutual interference between two or more such signals, and thereby to be able to select families of signals for which this mutual intereference is minimized. Mathematically, this is equivalent to developing a theory of the cross-correlation between two PN sequences of the same length.

II. Cross-Correlation of Binary Sequences

One approach to the cross-correlation problem which is applicable to any two binary PN sequences of the same period was developed by S. W. Golomb and published in [B,1] (which appeared in 1969). While this particular approach is very general and mathematically elegant, it does not yield quick or computationally simple solutions to the problem of selecting good collections of mutually compatible signals.

Another approach which has been developed primarily by Dr. Welch involves the theory of trace mappings in finite fields. By this method, it has been possible to show that if $A = \{a_i\}$ is a PN sequence, then $A' = \{a_{qi}\}$ is another PN sequence of the same period having minimal interference with the sequence A for certain specific values of q. These

include:

1) $q = 2^j + 1$ for $j = 1,2,3,\ldots$ and $(n,j) = 1$

2) $q = 4^j - 2^j + 1$ for $j = 1,2,3,\ldots$ and $(n,j) = 1$

3) $q = 2^{(n-1)/2} + 3$ for all odd

4) The multiplicative inverses, modulo $2^n - 1$, of any of the above values of q.

Collectively, these cases account for nearly all the observed instances in which the most favorable cross-correlation condition occurs, and it is possible to pick combinations from among these cases in order to obtain sets containing several mutually compatible signals.

The theoretical and experimental work to date involving the binary sequence case is being written up in a Ph.D. dissertation by a doctoral candidate Yoji Niho, under support furnished exclusively by this grant [A,3].

III. Cross-Correlation of Poly-Phase Sequences

The use of PN sequences over a p-phase alphabet greatly increases the options available to the communicator. The possibility of generalizing or modifying the results from the binary case so as to apply to the p-symbol alphabet has been the subject of a highly successful Ph.D. dissertation by Mr. Herbert Trachtenberg[A,1]. Mr. Trachtenberg's results include the optimality of cross-correlation between the sequences $A = \{a_i\}$ and $A' = \{a_{qi}\}$ for the cases

1) $q = \frac{p^j + 1}{2}$, n odd

2) $q = p^{2j} - p^j + 1$, n odd

3) The multiplicative inverses, modulo $p^n - 1$, of any of the above values of q.

Mr. Trachtenberg successfully defended his thesis, entitled "On the Cross-Correlation of Maximal Linear Shift Register Sequences", on December 6,

1969, and will receive the Ph.D. degree at the end of the current semester.

IV. Other Progress

Related problems in the understanding of shift register sequences have also been successfully studied, with the support of this grant. In particular, Mr. Harold Fredricksen wrote a successful Ph.D. dissertation entitled "Disjoint Cycles from the De Bruijn Graph", which expiores the question of the number of disjoint cycles which may be found in the state diagram of a shift register generator. Also, Dr. Abraham Lempel worked on these and related problems while a post-doctoral fellow at USC during 1968-1969, and his papers (B,3) and (B,4), acknowledging the support of this ARO-D grant, have been scheduled for publication.

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A. Theses Supported by this Grant

1. Harold Fredricksen, "Disjoint Cycles from the De Bruijn Graph".

2. Herbert Trachtenberg, "On the Cross-Correlation of Maximal Linear Shift Register Sequences".

3. Yoji Niho, "Patterns in Cross-Correlation".

B. Papers Acknowledging this Grant

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2. R. A. Scholtz and L. R. Welch, "The Mechanization of Codes with Bounded Synchronization Delays", Transactions on Information Theory, to appear.

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4. Abraham Lempel, "On Extremal Factors of the De Bruijn Graph", Journal of Combinatorial Theory, to appear.

3.3 SWITCHING, AUTOMATA THEORY, COMPUTERS

3.3.1 Automata and Formal Language Theory

GJ 454, National Science Foundation
AF-AFOSR 69-1622, Joint Services Electronics Program

R. Card, W. Chandler, S. Ginsburg

Background

During the past five years, a multitude of different types of acceptors and the langugages they recognize have been introduced. Recently, it was observed that most of these devices and languages would be subsumed and unified within the notions of an "abstract family of acceptors", abbreviated AFA, and an "abstract family of languages", abbreviated AFL. This has resulted in a flood of new questions and results, hitherto unsuspected. Whereas before the advent of AFA, there was a surfeit of devices, after AFA there was a sudden scarcity. This situation arose because there were not enough different types of extant devices to answer the new questions.

Progress

William Chandler concludes his study[1], described in the previous report period, of languages accepted by families of deterministic devices and has received his Ph.D.

Roger Card concluded his study[2] of associative memory acceptors and has received his Ph.D. In his thesis he examined associative memory acceptors under realtime operation. He showed that the family L of languages accepted by realtime memory acceptors properly contain the family of languages accepted by 1-tape realtime Turing

acceptors. In addition, he exhibited a family of languages in L, each accepted by no n-tape realtime Turing acceptor. He then proved that L contained an infinite hierarchy of realtime languages. Finally he obtained some counter examples to prove nonclosure results for certain families of the hierarchy.

A report entitled "Principal AFL" was written. A (full) principal AFL is a (full) AFL generated by single languages; i.e., it is the smallest (full) AFL containing the given language. In the paper, a study was made of such AFL. First, an AFA (abstract family of acceptors) characterization of (full) principal AFL was given. From this result, many well-known families of AFL can be shown to be (full) principal AFL. Next, a representation theorem for each languages in a (full) principal AFL was given involving the generator and one application each of concatenation, star, intersection with a regular set, inverse homomorphism, and a special type of homomorphism. Finally, it was shown that if $\mathcal{L}_1$ and $\mathcal{L}_2$ are (full) principal AFL, then so are (a) the smallest (full) AFL containing $\{L_1 \cap L_2/L_1$ in $\mathcal{L}_1$, L_2 in $\mathcal{L}_2\}$ and (b) the family obtained by substituting ϵ-free languages of $\mathcal{L}_2$ into languages of $\mathcal{L}_1$.

A report entitled "Images of AFL Under Certain Families of Homomorphism" was written. It was shown that a certain family of homomorphic images of sets is an AFL. A consequence of this result is that the images of sets is an AFL. A consequence of this result is that the images of linear-decreasing homomorphisms of sets in an AFL is an AFL.

A number of previous reports were either published[5,6,7] or accepted for publication[8,9].

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3.3.2 Fault Detection in Combinational and Sequential Networks

AF-AFOSR 69-1622A, Joint Services Electronics Program
GK 4386, National Science Foundation

M. A. Breuer

Background

An outstanding unsolved problem in switching theory deals with the generation of fault detection sequences for sequential machines. This problem can be simply stated as follows: Given the logical structure of a sequential machine M_o, and K hardware faults, say $k = 1, 2, \cdots, K$, each defining a machine M_k, where $M_k \neq M_o$; determine an input sequence $\underline{X}$ such that by observing the response one can determine whether or not the machine is M_o or M_k for some $1 \leq k \leq K$.

This problem has great practical importance. For example, current LSI technology now makes it possible to build circuit chips containing hundreds of flip flops and gates. These chips may contain from 30-50 input/output leads. Once these chips have been sealed, their internal components cannot be directly tested, hence their correct operation can only be determined via external testing. The efficient generation of these tests for all but the simplest circuits is an unsolved problem. Unless this problem can be solved, the applicability of these chips will be severely restricted. The aim of the research proposed here is to solve this testing problem.

One of the earliest results on detecting and diagnosing failures in sequential circuits was reported by Moore.[1] From a practical point of view Moore's approach is infeasible since it leads to extremely long test sequences. Hennie[2] was able to significantly shorten these test sequences by reducing the problem to that of only detecting a failure rather than diagnosing it. Finally, Kohavi[3] has shown that by adding additional output terminals the length of the test sequence can be further reduced. Of course, if we can inspect the output of every state device, then we can

reduce the problem to that of testing a pure combinational logic circuit, and the D-algorithm of Roth[4] can be applied. We will not consider this degenerate case.

Previous Accomplishments

(1) State Diagram Approach

We have investigated the following problem: Given the state transition description of a sequential machine and a set of faults each of which causes an error in the output as well as a possible error in the state transition. These faults can be detected by activating certain state transitions. A fault detection test sequence is then obtained by activating each of these transitions. We have developed an algorithm for constructing a minimal length fault detection test sequence.

(2) Cascaded Machines

Many sequential circuits can be decomposed into a sequence of n identical sequential circuits. This type of structure is quite common, e.g., most registers and accumulators fall into this category. This class of machines can be tested as n small circuits rather than as one large circuit. In fact, in some cases it is possible to test these n small circuits simultaneously. We have shown, however, that though this is usually not the case, it is possible to divide the n circuits into two groups of n/2 circuits and test each group simultaneously. These techniques lead to a very short test sequence.

We have developed a theory for the testing of cascaded identical machines. Most of these results have been reported in reference 5.

Present Work

Generation of fault tests for linear logic networks. Consider a combinational logic network C consisting of only linear (exclusive-or) logic elements. We can associate with this network a set K of faults, say of the type s-a-1 and s-a-0. We can easily study the fault properties of this network by introducing an error vector $\underline{E}(j) = (\alpha_1(j), \alpha_2(j), \ldots, \alpha_J(j))$

associated with faults on line j of C. The $\alpha_i(j)$, for lines i = 1,2,...,J of C are determined as follows. Set $\alpha_i(j) = 0$ for all primary input lines. Set $\alpha_j(j) = 1$. Simulate the logic for these initial conditions. The resulting line values define $\alpha_i(j)$ and hence $\underline{E}(j)$.

Let $v_i^k(x)$ be the value of line i in C when x is applied as an input and the k th fault is present. Let $\underline{V}^k(x) = (v_1^k(x), v_2^k(x), \ldots, v_J^k(x))$, where k=0 refers to the fault free circuit.

Theorem 1: If $v_j^o(x) = \bar{\delta}$ and fault k consists of line j s-a-δ, then

$$\underline{V}^k(x) = \underline{E}(j) \oplus \underline{V}^o(x) .$$

Hence $\underline{E}(j)$ characterizes how the effect of an initial signal error due to a fault propagates through the circuit.

Corollary: If $\alpha_i(j) = 0$ for every primary output line i, then gate j is redundant.

Assuming no redundancy in C, we have

Theorem 2: Input x will detect fault k(j s-a-δ) if and only if $v_j^o(x) = \bar{\delta}$.

Corollary: $x_1, x_2, \ldots, x_L$ is a complete fault test family with respect to all s-a-1 and s-a-0 faults if and only if for each line j in C and each choice of $\delta \in \{0,1\}$, there exists an x_ℓ such that $v_j^o(x_\ell) = \delta$.

The bounds on the minimal value of L are as follows. $L \geq 2$ if all gates in C have an odd number of inputs, otherwise $L \geq 3$. Finally, $L \leq J$.

We have extended these results to include the case of multiple faults and also fault diagnosis.

Future Plans

(1) Generation of Minimal Length Fault Detecting Sequences

By adding additional outputs it is known that we can reduce the length of the test sequence. Kohavi's technique is implemented via intuition

and trial and error. We plan on formalizing his techniques. The problem of generating minimal length distinguishing sequences given a fixed number of additional outputs can be formulated as a number of unsolved directed graph problems. Two of these which we plan on studying are:

(a) find the minimal length path in a directed graph which transverses each branch at least once.

(b) given a directed graph G, remove K branches such that the length of the longest path in the resulting graph is minimal.

(2) Probablistic Approach

In most cases it is not necessary to guarantee with probability one that M and M' are equivalent. There are two reasons for this. First the actual test sequence may be very long only because certain failures which are quite unlikely to occur must be checked for. Secondly, it is possible that a failure occurs after it has been checked for in which case it goes undetected. Hence, one problem which we will investigate is the generation of partial test sequences of a given length n which maximize the probability of detecting a failure. Both optimal and heuristic solutions to this problem will be sought. Finally, a theoretic study of the effectiveness of random input test sequences will be investigated.

(3) Test Generation Program

We are currently writing a program for generating fault tests for sequential machines. This program will implement a number of different strategies, such as random test generation, the D-algorithm, and a new concept referred to as the repeated state algorithm.

(4) Self Testing Circuits

A somewhat different approach to the testing problem is the design of circuits with self failure detecting circuitry. This may include the use of some redundant components and majority logic in order to increase the reliability of a circuit. However, the main objective here

is not really that of increasing system reliability as is so important in space borne computers, but rather the construction of circuits which detect their own faults. This problem has not been analyzed except for some specific circuits.

The interrelationships between improving the reliability of a circuit and its degree of testability needs to be investigated. From this analysis we hope to be able to learn how to effectively modify present circuit design techniques to include the concepts of reliability and testability.

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3.3.3 Hazards in Asynchronous Sequential Circuits

AF-AFOSR 67-1018B, Air Force Office of Scientific Research

W. S. Meisel and R. S. Kashef

Introduction

Practical electronic switching networks differ from theoretical networks largely in the presence of delay. Signals supposedly representing complements may temporarily take identical values.

As a result of this departure from the ideal, a switching circuit may operate incorrectly. A logical circuit in which delays may assume values which will cause this incorrect operation contains a "hazard". Due to such potential misbehavior in sequential ciricuits, research was carried out in order to find an algorithm which could be used for the detection and elimination of possible multiple-order hazards in sequential networks.

Unger founded the study of sequential hazards[3,4]. He gave an excellent discussion of the theory of designing a sequential circuit to prevent hazards when possible, assuming that upper and lower bounds on the delays are not available. One of his conclusions was that under these conditions, certain "essential" hazards could not be designed away and had to be corrected by delay.

The approach taken in this study was somewhat different with the assumptions being that (1) the sequential circuit has been designed by criteria other than hazards prevention (e.g., state minimization), and (2) both upper and lower bounds on delays are available.

Multiple-Order Hazards

An Asynchronous sequential circuit may be visualized as Fig. 1. The elimination of hazards in the outputs $z_1, \ldots, z_n$ is a combinational problem and was not considered. Furthermore, the following assumptions were made about the networks considered.

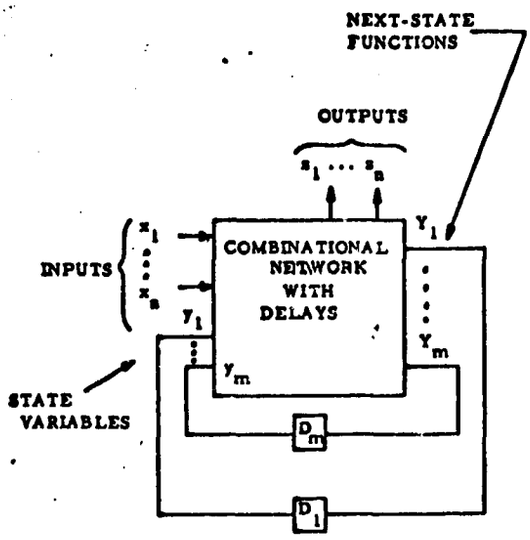

Fig. 1. Asynchronous sequentical circuit

1) Static and dynamic hazards do not occur in the feedback network.

2) Input variables change one at a time, and there is enough time between changes to allow the network to reach a stable state.

3) There are no races; that is, the flow table is coded so that all transitions between states involve only single changes of secondary variables, or a series of single changes.

By looking at the coded flow table, it was possible to derive an algorithm which provided the number and types of possible multiple-order hazards. Furthermore, by examining the circuit which realizes the coded flow table and the state equations used to implement the circuit it was possible to determine whether possible hazards could actually occur. If the hazard occurance could be determined, then an algorithm was provided which could be used to determine the bounds on the delays under which the hazard could occur. Figure 2 shows, symbolically, zero, first and second order hazards and the delay condition under which these could occur.

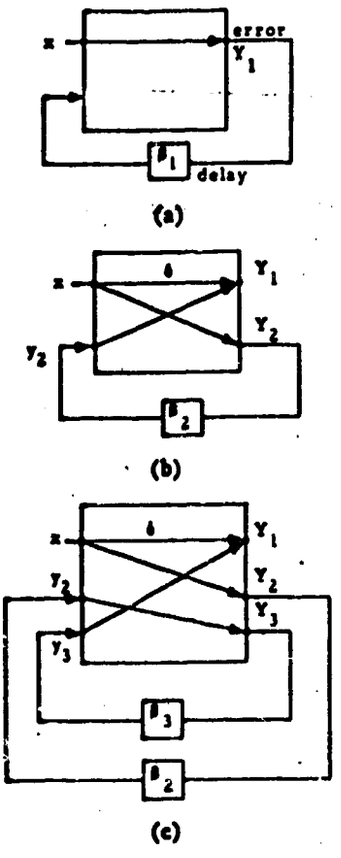

Fig. 2. (a) Zero-order hazard. Cannot be eliminated by increasing β_1. (b) First-order hazard. Possible error for $\delta > \beta_2$. (c) Second-order hazard. Possible error for $\delta > \beta_2 + \beta_3$.

The detailed result of this research can be found in reference 5.

The assumption that static and dynamic hazards do not occur in the feedback network motivates further research in detection and elimination of static and dynamic hazards. Extensive work done in this area thus far lacks both generality and correctness in all cases. Research is underway to extend the present results and provide a method by which possible static and dynamic hazards can be detected and corrected in case of actual occurance.

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3.3.4 Minimum Length Race-Free Coding for Asynchronous Sequential Machines

AF-AFOSR 67-1018B, Air Force Office of Scientific Research
AF-AFOSR 69-1622, Joint Services Electronics Program
R. S. Kashef

Due to an estimated large computer time required to complete the coding of 16-row tables with 5, 6, and 7 stable states, as reported in the previous progress report[1], a major modification, using sharing of coded paths, to the existing coding program was undertaken. Test runs thus far, using the modified program, indicated that coding time for the remaining tables will be reduced by a factor of 4. Further work is being carried out in order to prove that columns of 2^{S_o}-row flow tables, with S_o-even, whose states can be partitioned into 2^{S_o-1} pairs of maximum distance are the only columns which require the use of all 2^{n-S_o} unused code words among the set of all possible 2^n n-bit APC code words. This is being attempted by the use of graph theory approach for the case with $S_o = 4$.

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3.3.5 Theory of Cognitive Processes

NGR-05-018-044, National Aeronautics and Space Administration

W. S. Meisel and D. A. Michalopoulos

Introduction

The theory of cognitive processes has two aspects: (1) the attempt to understand human thought processes and (2) the design of a machine able to learn, conceptualize, and abstract. While complementary, these objectives must be approached from different points of view: it is neither sensible to view a human as a machine or to impose human characteristics upon a machine. The common link is the basic complexity necessary to both systems.

Self-Programming Computers

A self-programming computer (1) should operate from the specification of a task rather than an algorithm, (2) should retain from the execution of one task information to improve the execution of another, and (3) should be able to abstract from its retained experience means for the solution of new classes of problems or more efficient solution of old classes of problems.

One obvious raison d'etre for such a machine would be the programming (or verification of human programming) for complex computer-based systems upon which critical decisions may be based; there is presently no way of obtaining complete assurance that all aspects of the software of a complex system operate properly. (Consider the failure of the television network's vote collecting and tabulating system during the last Presidential election.) Another might be the improvement and invention of numerical methods. The basic power of the self-programming computer would presumably derive from its ability to solve a problem with only a vague problem specification and no specifics as to the means of solution. We wish a machine that is not oriented toward beating humans

at their own games, but one which does what humans do not do well.

Our aim in this discussion is not to present a finished design for a self-programming computer, but to give some concrete estimate of the feasibility of the prospect. Toward this end, some specific aspects of a possible design will be outlined.

Let there be N cost registers $c_1, c_2, \ldots, c_N$, where we will distinguish only by context between registers and the numerical contents of those registers. The numbers in the cost registers are calculated by different algorithms, using outputs of the computer and the environment (thus allowing evaluation by a teacher, be he human or machine). The built-in instinct of the computer is, in evaluating alternative actions, to choose that action which results in the smallest c_1, unless alternatives yield close values of c_1, in which case c_2 is similarly treated, and so on. (If none of the sequence provide a definitive comparison, the alternative minimizing c_1 is chosen.) This approach requires a task to be specified as a number of criteria, of varying importance, to be minimized. This is quite general, since each criteria can be a computer program in itself, and since the task need not be reduced to a single cost function.

The simplest way to approach the rationale behind choosing basic subsystems is to consider a typical sort of problem the computer might encounter. Suppose it wishes to minimize many multivariate functions $F(\underline{z})$ by the steepest descent technique with fixed step size:

$$\underline{z}_{i+1} = \underline{z}_i - \varepsilon \nabla F(\underline{z}_i) ; \qquad i = 1, 2, \ldots$$

Given F, how can the computer choose ε to get acceptably close to the minimum with the fewest iterations? Further, the machine must learn how to choose ε in the course of its normal work; it can only afford to minimize each function presented once. Hence, it cannot repeatedly test different ε's on a given function.

Figure 1 indicates a possible structure to handle this situation,

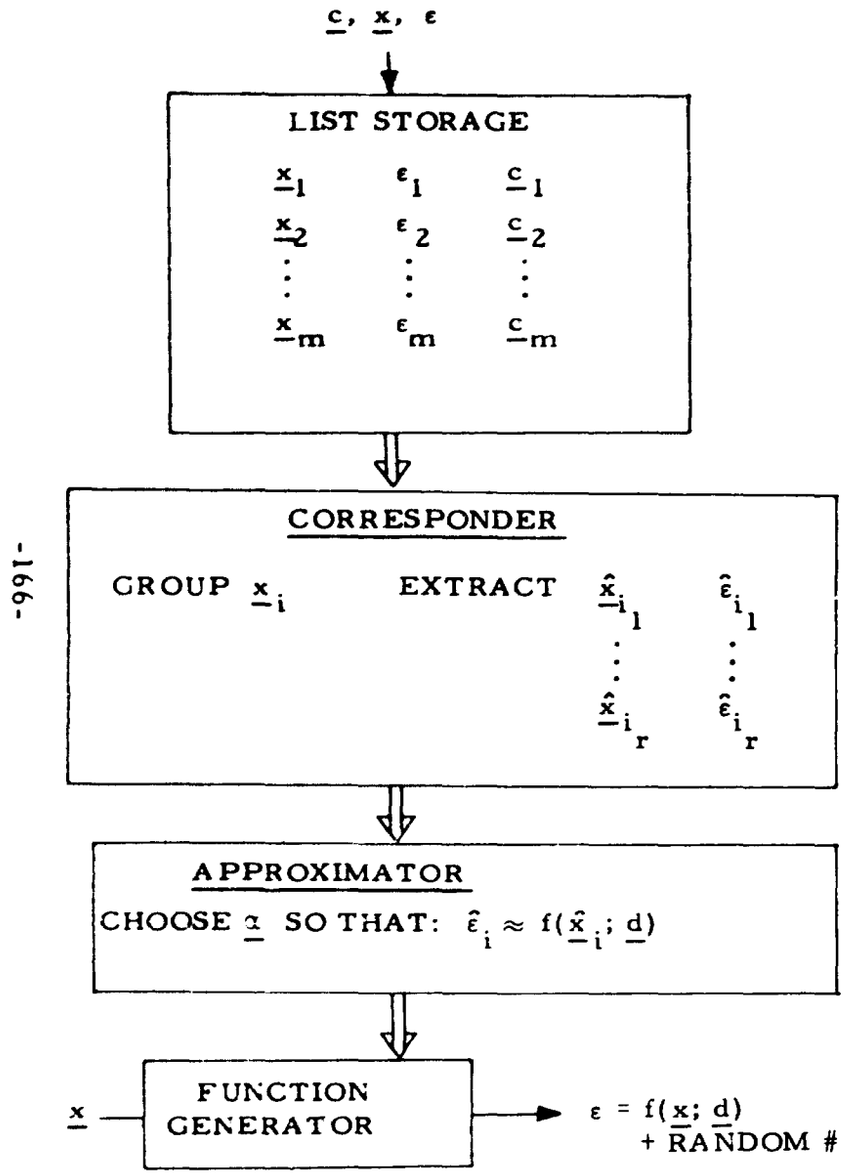


Figure 1

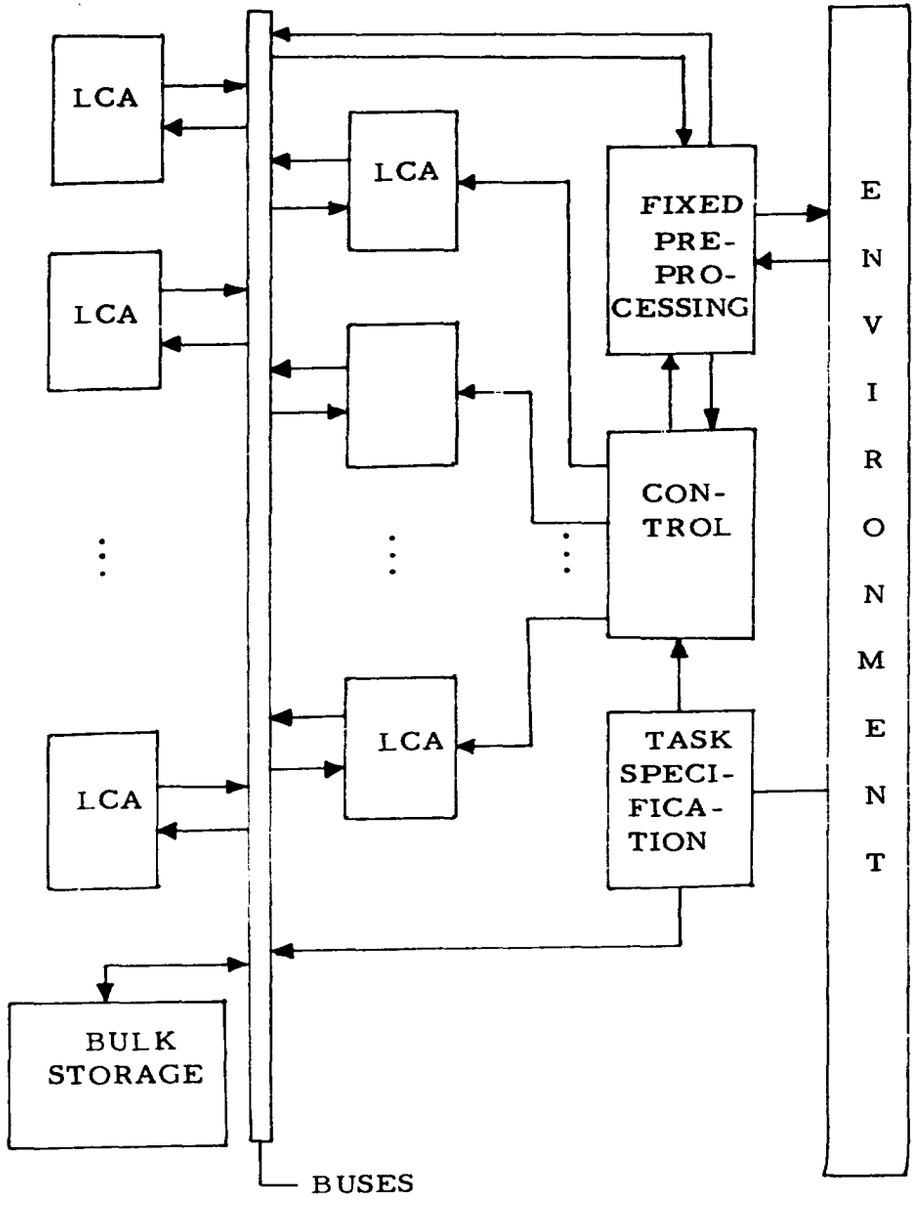


Figure 2

which we will unimaginatively denote a list-corresponder-approximator (LCA) unit. A function to be minimized is characterized by a relatively small number of scalars $x_1, \ldots, x_n$ representing features of the function relevant to the choice of ε. (For example, random lines could be drawn through $\underline{z}$-space, and statistics such as the average distance between local extremum on the lines calculated.) Whenever a function is minimized by the gradient technique, the value of ε is calculated by a function specified by the approximator and multiplied by a random number, the mean of which is 1 and the variance of which might decrease with time. The function $f(\underline{x})$ is parameterized, $f \equiv f(\underline{x}; \underline{\alpha})$, continuous in $\underline{x}$ and $\underline{\alpha}$ (e.g., a multivariate polynomial in $x_1, \ldots, x_n$ with coefficients $\alpha_1, \ldots, \alpha_R$); the system begins with some initial approximation.

The list storage collects experience: when it minimizes a function F_1 characterized by the feature vector $\underline{x}_1$, it stores $\underline{x}_1$ itself, the iteration constant ε_1 used in the process, and the cost vector $\underline{c}_1$ evaluating the performance. (In this case, c_1 could simply be the number of iterations.) It is assumed to be unlikely that a given function will appear twice in the sequence of functions presented to the computer. Hence, periodically, the corresponder interrogates the list storage and collects the $\underline{x}_i$ into small groups on the basis of their proximity in n-space. (Algorithms for this process are available as "cluster-seeking" or "subset generation" algorithms.) Each group so constructed should represent a set of similar functions. Suppose such a group with corresponding list entries is

$$\begin{array}{ccc} \underline{x}_{i_1} & \varepsilon_{i_1} & \underline{c}_{i_1} \\ \vdots & \vdots & \vdots \\ \underline{x}_{i_m} & \varepsilon_{i_m} & \underline{c}_{i_m} \end{array} .$$

Let $\hat{\underline{x}}_1$ be the mean of $\underline{x}_{i_1}, \ldots, \underline{x}_{i_m}$; let $\hat{\varepsilon}_1$ be the value of ε from the above list which is ranked best by the cost functions. Further suppose that this is done for every group:

$$\begin{matrix} \hat{\underline{x}}_1 & \hat{\varepsilon}_1 \\ \vdots & \vdots \\ \hat{\underline{x}}_r & \hat{\varepsilon}_r \end{matrix} .$$

Then $\hat{\varepsilon}_i$ is a good guess as to the best estimate to date of the value of ε to use for a function with characteristics similar to $\underline{x}_i$. Finally, the approximator generates a continuous function which satisfies $f(\hat{\underline{x}}_i) \approx \hat{\varepsilon}_i$, $i = 1,2,\ldots,r$. At any given time, the function f represents the cumulative experience of the computer.

Observations concerning this procedure follow:

(1) The random variation about $f(\underline{x})$ in the choice of ε is necessary or the computer will always generate an ε for a given $\underline{x}$ which falls on the initial approximation; hence, only minor modification of the initial function could ever be expected.

(2) List storage could be economized by "forgetting" points $\underline{x}_i$ which did not fall into groups over a long period of time or for which sufficient information had already been incorporated in $f(\underline{x})$.

(3) The corresponder could note the relative usefulness of the components of the feature vector in distinguishing clusters and feed back this information to the algorithms generating the features.

(4) The cost function need be specified only roughly. A further insensitivity to vagueness could be achieved by choosing the average ε corresponding to the two top-ranked values. Further, the cost functions need not be those for the overall task, but could be generated by the computer itself as a suboptimization problem within the overall task.

This subsystem is applicable to a wide range of problems and could be a fundamental component of a self-programming computer. If the parameterized algorithm were suitably general, a standardized unit could be replicated; the approximator should even be able to use other LCA units as subroutines. LCA units could generate features used by

other algorithms. They could specify cost functions. With appropriate interpretation of the inputs and outputs, they could indicate the order in which other algorithms should be executed.

Figure 2 indicates the interrelationship visualized between subsystems of the self-programming computer. The fixed pre-processing indicates the nature of the data and does any obvious pre-processing.

Reaction to the task specification is the function of the control unit. It may do so by using an LCA to choose the most appropriate LCA to order the use of the LCA's; it may repeatedly choose initial LCA units and compare their performance on the task specification, choosing the best. A structure which accomplishes this rudimentary function could be similar in structure to an LCA, but with more initial structure.

3.3.6 Mathematical Pattern Recognition

NGR-05-018-044, National Aeronautics and Space Administration

W. S. Meisel and W. W. Yuan

Introduction

The basic problems attacked by mathematical pattern recognition are those of (1) feature selection, extracting from a large set of measurements upon a physical system a greatly reduced set of numbers representing the information relevant to the recognition problem at hand, and (2) classification, classifying physical patterns into categories based upon the reduced representation obtained in the feature selection problem.

While solving what is a mathematical problem which can be formulated rather conretely, pattern recognition has suffered from its semantic implications. Evoking the image of the mimicking of humans, this field of study has often emphasized methods hypothesized as similar to human methods and applications challenging the human senses. By abandoning these emphases, by embracing computer-oriented techniques

and by turning more attention to patterns in data, mathematical pattern recognition is well along the way to becoming a set of engineering tools for application to a wide variety of problems--much as are mathematical programming and numerical analysis. They have promise in the study of many complex or poorly specified systems, systems for which we have empirical data but poor or non-existent models. Our research has been concentrated upon computer-oriented methods applicable to a wide range of problems.

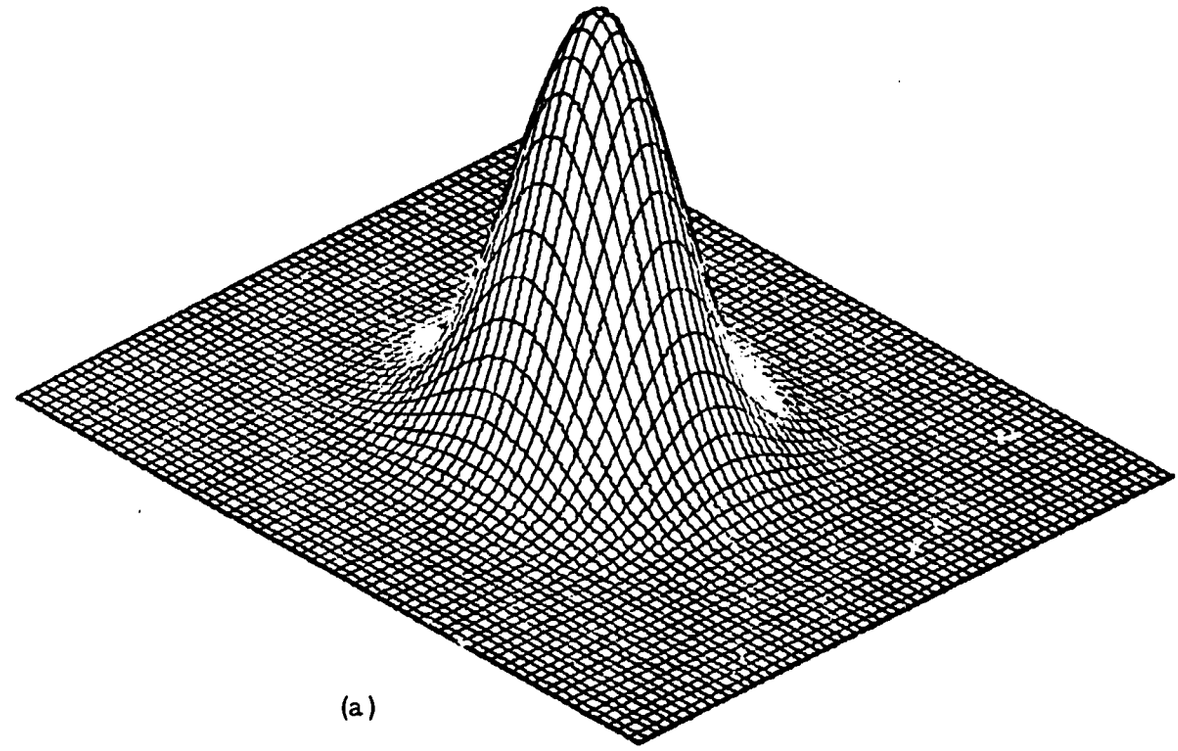
Constructive Pattern Classification Algorithms

There are two approaches to pattern classification[3,5]: (1) the definition of a cost function related to classification error of a set of samples and its minimization, and (2) the direct construction of discriminant functions for each class from samples of each class. The constructive approach has the advantage that it may be applied to a single class, indeed may often be interpreted as reconstructing an unknown joint probability density function from samples of a random process. The minimization approach is exemplified by linear discriminant functions and mean-square methods[1] and has historically received the loin's share of attention. Among constructive techniques are nearest-neighbor techniques and potential function methods[2,4,7]. Potential functions provide a common formalism for all constructive techniques; they are based upon the concept of measuring in a non-Euclidean sense the distance of a single point to be classified to a set of points of a given class. Figure 1b indicates a discriminant function which has been built up by the superposition of single potential functions of the form of figure 1a. We have attempted to emphasize the full generality and range of application of potential function methods[2,4].

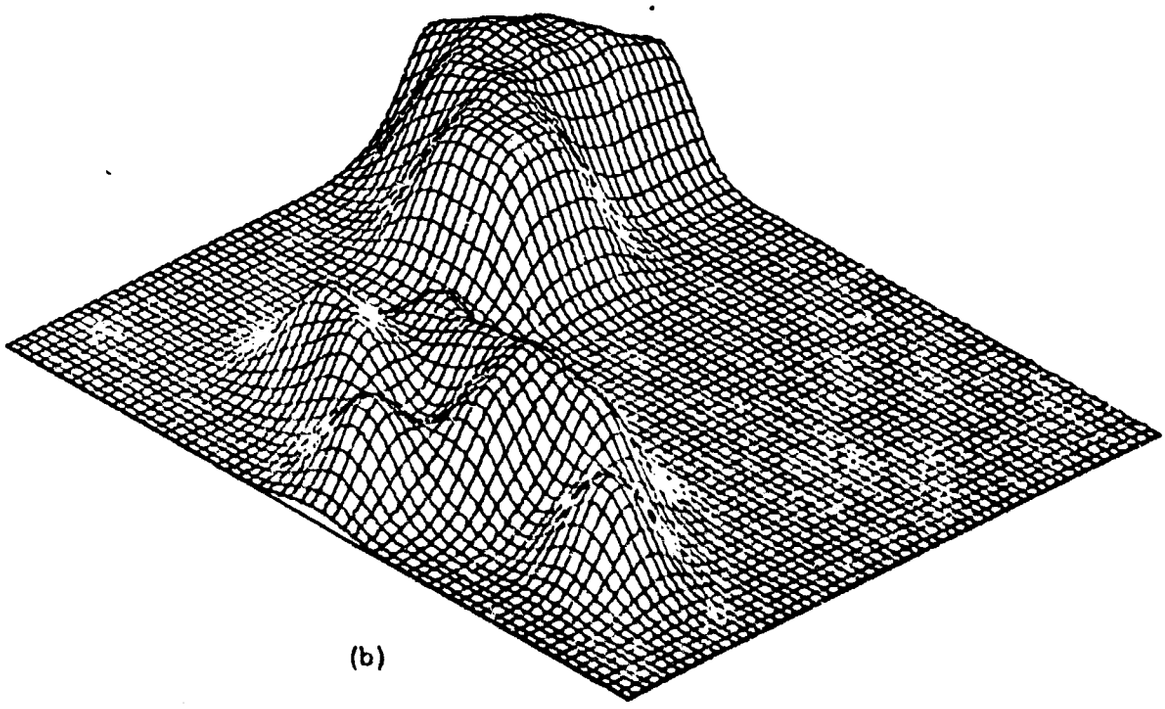
A major comparison of pattern recognition techniques upon artificial data has emphasized the power of constructive techniques[6].

Non-Stationary Patterns

We have formalized the concept of non-stationary patterns and demonstrated the implications of this formulation upon pattern classification



(a)



(b)

Figure 1

algorithms. We are continuing to refine this work in progress.

Feature Selection

An extension of concepts from potential function theory has provided some insights into the problem of choosing features for general multimodal distributions based upon samples of the process rather than upon heuristics.

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3. W. S. Meisel, Mathematical Pattern Recognition, (book in preparation).

4. W. S. Meisel, "Potential Functions in Pattern Classification Algorithms", Proc. 1969 Symposium on Adaptive Processes, November 1969.

5. W. S. Meisel, "Computer-Oriented Methods in Pattern Recognition", to be published.

6. W. S. Meisel and W. W. Yuan, "An Experimental Study of Pattern Classification Algorithms", to be published.

7. W. S. Meisel and Brian Schaeffer, "Low-Parameter Approximation", to be published.

8. W. S. Meisel and D. A. Michalopoulos, "Biased Random Search", to be published.

9. W. S. Meisel, "On the Design of Self-Programming Computers", presented at the Annual Meeting of the American Society for Cybernetics, Gaithersburg. Md., October 1969.

4. BIOMEDICAL ENGINEERING AND MATHEMATICS

4.1 RESEARCH PROJECTS IN BIOMEDICAL ENGINEERING

PO 1 GM 16437-02; 5805 FRO7012-03; 1F03GM 43984-01; 2FO3GM39547-02: Department of Health, Education and Welfare (USPHS)

F. S. Grodins, L. B. Wolf, G. P. Moore, F. E. Yates, A. V. Phatak and G. A. Bekey

4.1.1 Control of Breathing

F. S. Grodins, G. A. Bekey, S. Yamashiro and J. D. Smith

By means of experimental work on animals, and a parallel computer simulation with hybrid techniques the design principles of the respiratory mechanical system are being described. The system has at least two levels of control, one concerned with adjusting the average level of lung ventilation in order to maintain normal values of oxygen and carbon dioxide in blood, and the other with choosing a pattern for the respiratory cycle that will yield this average level with a minimum "mechanical cost". This project has also led to an extension in modeling technique itself.

4.1.2 Studies of the Fetal Cardiovascular System

G. A. Bekey

A mathematical model of the fetal cardiovascular system has been developed and simulated on a computer. Its behavior has been compared to that observed experimentally in the near-term fetal lamb. The study led to the conclusion that control loops exist in the fetus which operate upon the vascular conductance of the placental circuit. Thus, the unborn animal has means to adjust placental blood flow in support of mass

transfer processes occurring in that organ.

4.1.3 Design of Artificial Kidneys

M. B. Wolf and R. Kalaba

This study is aimed at understanding the complex processes by which the kidney regulates a large number of substances in the blood within limits compatible with life, and with the application of this knowledge to improve the basic theory of artificial kidney therapy. A mathematical model of the patient-artificial kidney system has been developed which enables the physician to predict the effects of dialysis that will be achieved by given parameter settings in the apparatus. Modern mathematical control theory is being used to "optimize" the treatment regime.

4.1.4 Endocrine Signals and Systems

F. E. Yates, J. Urquhart, A. V. Phatak

By means of programmed infusions achieved through the coupling of laboratory computers to servopumps, metabolic systems are forced with sin, step, pulse, ramp or pseudorandom functions in order to characterize component and system dynamics. The systems under study include the global adrenal glucocorticoid system (studied in unanesthetized dogs), and the isolated, perfused dog liver. In each case, input/output relationships are obtained for a variety of initial conditions and operating levels. Computer simulation based upon postulated system structure is used for interpretation of the data. Emphasis is placed on the nature of information flow, communication and control in the chemical processing that underlies energy conversions in animals.

4.1.5 Models of Neuronal Activity

G. P. Moore, J.H. Penaloza-Rojas, H. Sugiyama,
R. J. Sclabassi and J. L. Gehrich

Encouraging new results have been obtained in the last half-year both in the experimental and theoretical study of small neuronal networks.

In one project (undertaken by Mr. R. J. Sclabassi as a Ph.D. dissertation) signals from a specific area of the brain concerned with sensory information processing have been analyzed and a theory explaining the pattern of activity has been advanced[1]. In addition, computer programs have been completed which greatly expand our data-processing capabilities for neuronal signals and we now have both simulation, parameter estimation routines to go with the processing packages.

Mr. J. L. Gehrich is continuing his doctoral studies on mathematical and computer models of discharge patterns in chemical-sensitive nerve cells which form part of the feedback pathway in the control of breathing[2].

With Professor Sugiyama, visiting from Osaka University, we have completed a theoretical study of random-walk models of neuronal signals and this will appear shortly[3]. In this work, Professor Sugiyama has succeeded in obtaining analytical and numerical solutions to the first passage problem of a random-walk model of the neuron which is of sufficient generality to apply to a large number of neuronal networks.

In addition, work has been completed on a major effort concerned with the use of statistical techniques to detect and characterize neuronal interactions. We hope that this work, to be submitted for publication, will provide powerful techniques for the study of nerve network structures[4]. Effective use of these techniques in the study of the network organization of visual centers of the cat brain has already been made[5].

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2. Gehrich, J. L. and G. P. Moore, "Theoretical Models of Chemoreceptor Discharge Patterns", to be presented at the 7th Annual Meeting Engineering Sciences in Biomedicine, Washington University, St. Louis.

3. Sugiyama, H., G. P. Moore and D. H. Perkel, "On Some Random-Walk Models for Neuronal Spike Trains", (in press).

4. Moore, G. P., J. P. Segundo, D. H. Perkel and H. Levitan, "Statistical Signs of Synaptic Interactions in Neurons", to be published.

5. Moore, G. P., J. H. Penaloza-Rojas and B. Okamura, "Models of Nerve Cell Interactions in the Cat Visual System", Proc. Int. Cybernetics Congress, Lodon, 1969, (in press).

4.2 MATHEMATICS IN BIOLOGY AND MEDICINE, NONLINEAR ANALYSIS AND RADIATIVE TRANSFER

GM 16197-01, GM 16197-02, Department of Health, Education and Welfare (USPHS)

GF 294, GP-8960, National Science Foundation

AT(11-1)-113 Project #19, Atomic Energy Commission

R. Bellman and others cited in subsections

4.2.1 Chemotherapy and Drug Administration

One of our major areas of research continues to be chemotherapy, with particular emphasis upon pharmocokinetics and the clinical administration of drugs. June Buell and Robert Kalaba are pursuing their close collaboration with Dr. Roger Jelliffe, of the USC-LAC Medical Center in connection with the administration of digitalis and other drugs.

The mathematical investigations center about three aspects: descriptive, control, and identification. By descriptive we mean a numerical prediction of the consequences of certain biochemical assumptions; by control we mean a determination of the drug regimen that will produce desirable results, by identification we mean a determination of biochemical patient parameters so that effective dosage can be administered.

Recent results are contained in

Jelliffe, R., J. Buell, R. Kalaba, R. Sridhar, and R. Rockwell, A Mathematical Study of the Metabolic Conversion of Digitoxin to Digoxin in Man, USCEE-347, April 1969; to appear in Mathematical Biosciences.

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Buell, J., R. Kalaba and M. B. Wolf, A New Approach to Transients in Countercurrent Flow Systems, Technical Report 69-22, October 1969.

4.2.2 Identification of Systems

The determination of the internal structure of systems on the basis of convenient, inexpensive, and painless observations continues to be another of our major directions of research.

Recent work is contained in

Bellman, R., A New Method for the Identification of Systems, USCEE-337, March 1969; Mathematical Biosciences, Vol. 5, 1969, pp. 201-204.

Angel, E., Inverse Boundary-Value Problems: Elliptic Equations, USCEE-343, April 1969.

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Bellman, R., Topics in Pharmacokinetics--II: Identification of Time-Lag Processes, USCEE-367, June 1969; to appear in Mathematical Biosciences.

Friedland, S. S., The In-Vivo Use of Beta Emitting Isotopes and Silicon Semiconductor Detectors in Nuclear Medicine and Biology, USCEE-372, October 1969.

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Bellman, R., and H. Sugiyama, Identification of Parameters in Certain Stochastic Systems-I, Technical Report 69-15, October 1969.

4.2.3 Neurophysiology

We have two principal activities in the field of neurophysiology; the research of D. Trujillo in occasional collaboration with H. M. Lieberstein, and that of H. Sugiyama in collaboration with G. Moore and D. Perkel.

Recent work is contained in

Kaplan, S., and D. Trujillo, Numerical Studies of the Partial Differential Equations Governing Nerve Impulse Conduction--The Significance of Lieberstein's Inductance Term, USCEE-351, April 1969.

Moore, G., D. Perkel and H. Sugiyama, Random Walk Models for Neuronal Spike Train Production, Technical Report 69-9, October 1969.

4.2.4 Psychodynamics

We are actively continuing our efforts in psychodynamics. One of our objectives is to rewrite the computer program described in R. Bellman, M. B. Friend, and L. Kurland, "A Simulation of the Initial Psychiatric Interview", The RAND Corporation, R-449-RC, 1966,
--------, "On the Construction of a Simulation of the Initial Psychiatric Interview", Behavioral Sciences, Vol. 11, 1966, pp. 389-399,
--------, "A Simulation of the Initial Psychiatric Interview: Revised and Expanded Version", USCEE 240, December 1967,
so as to make it available for CRT (cathode ray tube) display, rather than the original typewriter format which possesses a number of disadvantages. This work, carried out by R. Luthardt and R. Reynolds, is now finished.

P. Kell, R. Bellman, and W. Hopgood, consultant, are preparing a library of short computerized simulations (vignettes) covering a wide range of situations encountered in initial interviews. K. Colby, Stanford University, consultant, is assisting in this effort. A detailed discussion of what is involved in this is contained in: R. Bellman, W. Hopgood, and P. Kell, "On the Construction of Simulations of Parts of the Initial Psychiatric Interview--I." This covers Case I of a list of

eight cases for which detailed writeups of the others will follows. This material will form part of a book by Bellman and Kell entitled Decision Making and Psychiatry, to be published by Basic Books in a series edited by Dr. Werner Mendel of the USC Medical School.

Recent work is contained in

Bellman, R., P. Kell, and W. C. Hopgood, "On the Construction of Vignettes: Short Simulation Processes for Role-Playing Purposes", USCEE-365, June 1969.

-----, "Computer Vignettes-I: The Young Psychiatrist," Technical Report 69-19, October 1969.

4.2.5 Auxiliary Mathematical Research

A major part of our program is the development of analytic and computational techniques for the solution of complex functional equations of the type that arise with frequency in biomedical research. In addition to the research that is sponsored by the NIH, we have support from the Atomic Energy Commission and the National Science Foundation, (two grants), for mathematical research of closely connected nature. For example, one of the major problems that ties mathematical physics and invariant imbedding to our mathematical biosciences program is the study of the effect of radiation upon human tissue and conversely the use of various radiation patterns for the location of tumors, etc. This is part of the general identification problem. The work that E. Angel, D. Collins, and A. Lew have been doing in the solution of potential equations is aimed at a number of diagnostic problems in the field of cardiology and chemotherapy.

A principal difficulty, particularly in control processes that arise in prosthetics and orthotics and drug administration, is that of "dimensionality." Even with the best of modern computers, high-dimensional systems of ordinary differential equations, differential-difference equations, and partial differential equations present severe difficulties as far as numerical solution is concerned. Considerable

progress has been made in this area. Results are contained in

McNabb, A., and A. Schumitzky, Factorization of Integral Operators--II: A Nonlinear Volterra Method for Numerical Solution of Linear Fredholm Equations, USCEE-330, March 1969.

Kalaba, R., and E. Ruspini, Invariant Imbedding and Potential Theory, USCEE-335, March 1969.

Bellman, R., H. Kagiwada, R. Kalaba, and S. Ueno, Diffuse Reflection of Solar Rays by a Spherical Shell Atmosphere, USCEE-348, April 1969.

Buell, J., R. Kalaba, and E. Ruspini, Numerical Results for a Mixed Boundary-Value Problem of Potential Theory Using Invariant Imbedding, USCEE-346, April 1969.

Collins, D.C., Terminal State Dynamic Programming: Quadratic Costs, Linear Differential Equations, USCEE-370, July 1969.

McNabb, A., and A. Schumitzky, Factorization of Operators--III: Initial Value Methods for Linear Two-Point Boundary Value Problems, USCEE-371, July 1969.

McNabb, A., and A. Schumitzky, Factorization of Operators--I: Algebraic Theory and Examples, USCEE-373, July 1969.

Collins, D., Reduction of Dimensionality in Dynamic Programming Via the Method of Diagonal Decomposition, USCEE-377, August 1969.

Collins, D., and A. Lew, Dimensional Approximation in Dynamic Programming: Application of Structural Decomposition to Differential-Difference Control Problems, Technical Report 69-3, September 1969.

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Collins, D., and A. Lew, Dimensional Approximation in Dynamic Programming: Application of Structural Decomposition to the Optimal Control of Diffusion Processes, Technical Report 69-5, September 1969.

Buell, J., J. Casti, R. Kalaba and S. Ueno, Exact Solution of a Family of Matrix Integral Equations for Multiply Scattered Partially Polarized Radiation--II, Technical Report 69-6, September 1969.

Kagiwada, H., R. Kalaba, and Y. Thomas, Exact Solution of Pontryagin's Equations of Optimal Control--I, Technical Report 69-7, September 1969.

Mathematical results covering a range of problems are contained in

Bellman, R., A Note on the Asymptotic Behavior of Solutions of Nonlinear Differential Equations, USCEE-344, April 1969; to appear in J. Math. Anal. Appl.

Kalaba, R., and E. Ruspini, Invariant Imbedding and Radiative Transfer in a Homogenous Cylindrical Medium, USCEE-349, April 1969.

Lew, A., Reduction of Dimensionality by Approximation Techniques: Diffusion Processes, USCEE-350, April 1969.

Odanaka, T., Analytic and Computational Studies of Optimal Inventory Processes--I: Approximation of Quantity, USCEE-352, April 1969.

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Wilcox, R. M., Closed-Form Solution of the Differential Equation ... by Normal Ordering Exponential Operators, USCEE-354, April 1969.

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Kagiwada, H., and R. Kalaba, Exact Solution of a Family of Integral Equations of Anisotropic Scattering, Technical Report 69-10, September 1969.

APPENDIX A

Publications

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"Application of Fourier-Hadamard Transformation to Bandwidth Compression", with W. K. Pratt, M.I.T. Symposium on Picture Bandwidth Compression, April 1969.

"Transform Data Coding", with W. K. Pratt, P.I.B. Symposium on Computer Processing in Communication, April 1969.

"Kronecker Matrices, Computer Implementation and Generalized Spectra", with J. Kane, to be published JACM.

"Decision Making and Pattern Recognition of Multi-Dimensional Data", IEEE-GMMS ERS International Symposium on Man-Machine Systems, September 8-12, 1969, Cambridge, England.

Computer Techniques in Image Processing, to be published, Academic Press.

"A Generalized Technique for Spectral Analysis", with K. L. Caspari, to be published, IEEE Transactions on Computers.

"Algorithmic Generation of a Class of Fast Transformations for Generalized Spectral Analysis", Hawaii International Conference on System Sciences, January 1970.

Bekey, G. A.

"Estimation of the Parameters of Sampled-Data Systems by Means of Stochastic Approximation", with C. B. Neal, Proc. Joint Automatic Control Conf., pp. 977-978, 1969.

"Mathematical Model of the Baroreceptor Reflex in the Full-Term Fetus", with W. Morrison and N. S. Assali, Proc. 8th Internationl Conference on Medical and Biological Engineering, pp. 20-24, 1969.

"A Model of the Adaptive Behavior of the Human Operator in Response to a Sudden Change in the Control Situation", with A. V. Phatak, IEEE Trans. on Non-Machine Systems, v. MMS-10, pp. 72-80, September 1969.

"On Modelling the Adaptive Characteristics of Human Controllers", Proc. Conf. on Applications of Continuous System Simulation Languages, (San Francisco), pp. 159-173, 1969.

Bellman, R.

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